Linear response and experimental measurements

As we have seen, for thermodynamic measurements, quantities involved are averages of operators at equal times.

For instance, the specific heat

$$C_V = \frac{dU}{dT} \qquad U = \langle H \rangle = \frac{\mathrm{Tr}\, H e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}}$$

$$\therefore -\frac{\partial U}{\partial \beta} = \langle H^2 \rangle - \langle H \rangle^2 = -\frac{\partial U}{\partial T}\frac{\partial T}{\partial \beta} = k_B T^2 C_V$$

$$\therefore C_V = \frac{1}{k_B T^2} \langle (H - \langle H \rangle)^2 \rangle = \frac{1}{k_B T^2} \langle (\Delta H)^2 \rangle$$

which is essentially the average of H^2, $\langle H(t) H(t) \rangle$, i.e., average of H at equal times.

Similarly, the magnetic susceptibility,

$$\chi = \lim_{h \to 0} \frac{M(h)}{h} = \frac{\partial M}{\partial h}\Big|_{h \to 0}$$

h = magnetic field
M = magnetization.

is also a thermodynamic measurement:

$$M(h) = \frac{\mathrm{Tr}\, M e^{-\beta(H - Mh)}}{\mathrm{Tr}\, e^{-\beta(H - Mh)}}$$

$$\left.\frac{\partial M}{\partial h}\right|_{h=0} = \langle \beta M^2 \rangle - \beta \langle M \rangle^2$$

$$\therefore \quad \chi k_B T = \langle (M - \langle M \rangle)^2 \rangle$$

which is essentially the average of M^2 at equal times.

In general, quanties in thermodynamics are averages of operators in equilibrium, $\langle O \rangle = \frac{\operatorname{Tr} O e^{-\beta H}}{\operatorname{Tr} e^{-\beta H}}$, hence all the measurements correspond to averages in equal times.

Linear response & the general Kubo formula

To go beyond thermodynamic measurements, one applies a time-dependent field (such as the electric field $\vec{E}(r,t)$ or the magnetic field $\vec{B}(\vec{r},t)$) and measures the response.

In real experiments, the field is applied at some starting t_0. Before t_0, the system is in equilibrium

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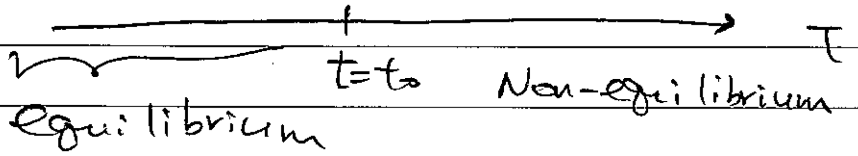
$\therefore H(t) = H_0 + H'(t)\, \theta(t-t_0)$



The key point of this setup is that the weight (probability) is given by the Boltzman distribution of H_0.

That is the density matrix $\hat{\rho}(t) = U(t,t_0)\,\hat{\rho}(t_0)\,U^{\dagger}(t_0,t_0)$

$$= U(t,t_0) \sum_n |n\rangle\langle n|\, e^{-\beta E_n}\, U^{\dagger}(t,t_0)$$

$$= \sum_n |n(t)\rangle \langle n(t)|\, e^{-\beta E_n}$$

where $H(t)|n(t)\rangle = i\hbar \frac{d}{dt}|n(t)\rangle$ and $H_0|n(t_0)\rangle = E_n|n(t_0)\rangle$

Then, the average of an observable at t is

$$\langle \hat{O}(t) \rangle = \frac{1}{Z_0} \mathrm{Tr}[\rho(t)\,\hat{O}]$$

$$= \frac{1}{Z_0} \sum_n \langle n(t)|\hat{O}|n(t)\rangle\, e^{-\beta E_n}$$

where $Z_0 = \sum_n e^{-\beta E_n}$.

In the interaction picture, one has

$$|n_I(t)\rangle = e^{\frac{iH_0t}{\hbar}}\,|n(t)\rangle$$

$$= U_I(t,t_0)\,|n_I(t_0)\rangle$$

$$\hat{O}_I(t) = e^{\frac{iH_0t}{\hbar}}\,\hat{O}\,e^{-\frac{i}{\hbar}H_0t}$$

and $$U_I(t,t_0) = T\,e^{-\frac{i}{\hbar}\int_{t_0}^{t} H_I'(t')dt'}$$

$$= 1-\frac{i}{\hbar}\int_{t_0}^{t} H_I'(t')\,dt' + \cdots$$

Hence, to linear order in H', one gets

$$\langle\hat{O}(t)\rangle = \frac{1}{Z_0}\sum_n \langle n_I(t)|\,\hat{O}_I(t)\,|n_I(t)\rangle\, e^{-\beta E_n}$$

$$|n_I(t)\rangle = |n_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} H_I'(t')\,dt'\,|n_I(t_0)\rangle + \cdots$$

$$\langle\hat{O}(t)\rangle = \langle O\rangle_0 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\langle[\hat{O}_I(t), H_I'(t')]\rangle_0\, dt' + \cdots$$

where $$\langle O\rangle_0 = \frac{1}{Z_0}\sum_n \langle n_I(t_0)|\,\hat{O}_I(t_0)\,|n_I(t_0)\rangle\, e^{-\beta E_n}$$

∴ To linear order, one gets

$$\delta\langle\hat{O}(t)\rangle \equiv \langle\hat{O}(t)\rangle - \langle O\rangle_0$$

$$= \int_{t_0}^{\infty} dt'\; C^R_{OH'}(t,t')$$

$$C^R_{OH'} = \frac{-i}{\hbar}\,\theta(t-t')\,\langle[\hat{O}_I(t), \hat{H}_I'(t')]\rangle_0$$

This is the general Kubo formula.

In general, H' is caused by external fields F(r,t) that couples to $\hat{O}$ linearly as

$$H' = \int dr\, \hat{O}(r,t)\, F(r,t)$$

$$\therefore\ H_I' = \int dr\, \hat{O}_I(r,t)\, F(r,t)$$

In this case, one gets

$$\delta\langle \hat{O}(r,t)\rangle = \int d\vec{r}\,' \int_{t_0}^{\infty} dt'\, \frac{-i}{\hbar}\,\theta(t-t')\,\langle[\hat{O}_I(r,t), \hat{O}_I(r',t')]\rangle_0 \times F(r',t')$$

$$\equiv \int d\vec{r}\,' \int_{t_0}^{\infty} dt'\, D^R(rt, r't')\, F(r',t') \quad --- ①$$

$$D^R(rt, r't') = \frac{-i}{\hbar}\,\theta(t-t')\,\langle[\hat{O}_I(rt), \hat{O}_I(r't')]\rangle_0$$

$$= \frac{-i}{\hbar}\,\theta(t-t')\,\langle[\hat{O}_H(rt), \hat{O}_H(r't')]\rangle_0 \quad --- ②$$

↑ ↗ Heisenberg picture

is called the linear response function.

From eq① & ②, it's clear that D^R is a retarded Green's function of the observable $\hat{O}$. Most importantly, even though observables involved are at different times, the average is w.r.t. equilibrium state!. Hence the linear response is determined by the equilibrium state !

Kubo formula for Conductivity

One of the most important quantities for the linear response is the conductivity (or resistivity).

In the original Landau theory of phase transitions, the order parameter is a thermodynamic quantity (parameter).

It is now realized that the order parameter can be more general. For metal - insulator transition, obviously, conductivity / resistivity is the order parameter, which is not a thermodynamic quantity !

If $\hat{O} = J_\alpha(r,t)$ α component of momentum density,

$\hat{O}$ is excited by external electric field

$$\vec{E}(\vec{r},t) = -\nabla \phi_{ext}(\vec{r},t) - \partial_t \vec{A}_{ext}(\vec{r},t) .$$

$$H' = -e\int dr\, n(r)\, \Phi_{ext}(\vec{r},t) + e\int d\vec{r}\, \vec{J}(r)\cdot\vec{A}_{ext}(\vec{r},t)$$

where Φ_{ext} & $\vec{A}_{ext}$ are external scalar & vector potential.

The momentumdensity, however, depends on the total vector potential $\vec{A} = \vec{A_0} + \vec{A}_{ext}$ with $\vec{A_0}$ being the vector potential in equilibrium.

$$\vec{J}(r) = \sum_{\sigma}\left\{\frac{1}{2m}\psi_\sigma^{+}\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)\psi_\alpha + \frac{1}{2m}\left[\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)\psi_\sigma\right]^{+}\psi_\alpha\right\} \quad (\vec{J}^{+} = \vec{J})$$

$$= \underset{\overset{\uparrow}{\times e = \text{paramagnetic current}}}{\vec{J_P}(\vec{r})} + \vec{J_D}(\vec{r}) \leftarrow \overset{\times e}{=} \text{diamagnetic current}$$

$$\vec{J_P}^{\sigma} = \frac{\hbar}{2mi}\left(\psi_\sigma^{+}\nabla\psi_\sigma - (\nabla\psi_\sigma^{+})\psi_\sigma\right) \qquad \vec{J_P} = \vec{J_P}^{\uparrow} + \vec{J_P}^{\downarrow}$$

$$\vec{J_D}^{\sigma} = -\frac{q}{m}\vec{A}(\vec{r})\,\psi_\sigma^{+}\psi_\sigma \qquad \vec{J_D} = \vec{J_D}^{\uparrow} + \vec{J_D}^{\downarrow}$$

$$\therefore \vec{J}(\vec{r}) = \vec{J_P} + \frac{e}{m}\vec{A}(\vec{r})\,n(\vec{r})$$

$$= \underbrace{\vec{J_P} + \frac{e}{m}\vec{A_0}\,n(\vec{r})}_{\to J_0(\vec{r})} + \frac{e}{m}\vec{A}_{ext}\,n(r)$$

Now, by suitable choosing gauge, one can set $\phi_{ext} = 0$ so that $\vec{A}_{ext}(r,\omega) = \frac{1}{i\omega}\vec{E}(\vec{r},\omega)$.

To linear order of $\vec{A}_{ext}$, one gets

$$H' = \frac{e}{i\omega}\int dr\, \vec{J}(\vec{r}) \cdot \vec{E}_{ext}(r,\omega)$$

$$\cong \frac{e}{i\omega}\int dr \left(\vec{J_P} + \frac{e}{m}\vec{A_0}\,n(\vec{r})\right) \cdot \vec{E}_{ext} + \text{higher order}$$

Making use of the linear response theory,

$$\therefore \langle \vec{J}(\vec{r},\omega)\rangle = \langle \vec{J_0}(\vec{r},\omega)\rangle + \frac{e}{m}\vec{A}_{ext}(r,\omega)\,\langle n(r,\omega)\rangle$$

$$= \langle \vec{J}_0(r,\omega) \rangle + \frac{e}{m} \vec{A}_{ext}(r,\omega) \langle n(r,\omega) \rangle_0 + \cdots$$

$$\delta \langle J_0^{\alpha}(r,\omega) \rangle = e \int dr' \sum_{\beta} \Pi^R_{\alpha\beta}(r,r',\omega) A^{\beta}_{ext}(r',\omega)$$

where $\Pi^R_{\alpha\beta}(rt; r't') = -i\theta(t-t') \langle [J_0^{\alpha}(rt), J_0^{\beta}(r't')] \rangle_0$

$$\therefore \delta \langle J_{\alpha}(r,\omega) \rangle = \int dr' \sum_{\beta} \left[e\Pi^R_{\alpha\beta}(r,r',\omega) + \frac{e}{m} \delta_{\alpha\beta} \langle n(r,\omega) \rangle_0 \right] A^{\beta}_{ext}(r',\omega)$$

$$= \int dr' \sum_{\beta} \left[\frac{\mp ie}{\omega} \Pi^R_{\alpha\beta}(r,r',\omega) + \frac{e\langle n \rangle_0}{i\omega m} \delta_{\alpha\beta} \right] E^{\beta}(r',\omega)$$

$\because$ Electric current density $\vec{J}_e = (-e) \langle \vec{J} \rangle$

$\therefore$ One gets

$$\delta \langle J^e_{\alpha}(r,\omega) \rangle = \int dr' \left[\sum_{\beta} \frac{-i}{\omega} \Pi^R_{\alpha\beta}(r,r',\omega) - \frac{e^2}{i\omega m} \langle n \rangle_0 \delta_{\alpha\beta} \right] E^{\beta}(r',\omega)$$

where $\Pi^R_{\alpha\beta} = -i\theta(t-t') \langle [J_{e0}^{\alpha}(rt), J_{e0}^{\beta}(r't')] \rangle_0$

$$\underset{\substack{\uparrow \\ \text{if } A_0 \text{ in equilibrium} = 0}}{=} -i\theta(t-t') \langle [J_p^{\alpha}(r,t), J_p^{\beta}(r',t')] \rangle_0$$

One identifies

$$\sigma_{\alpha\beta}(r,r',\omega) = \frac{+i}{\omega} \left[\Pi^R_{\alpha\beta}(r,r',\omega) + -e^2 \frac{\langle n \rangle_0}{m} \delta_{\alpha\beta} \right]$$

as the conductivity tensor.

In the momentum space, one gets

$$G_{\alpha\beta}(q,\omega) = \frac{i}{\omega}\left[\Pi^R_{\alpha\beta}(q,\omega) + \frac{e^2}{m}\langle n\rangle_0\,\delta_{\alpha\beta}\right] \quad --- ①$$

with $$\Pi^R_{\alpha\beta}(q,\omega) = \frac{-i}{V}\int_{-\infty}^{\infty} dt\,\theta(t-t')\,e^{i\omega(t-t')}\langle[J^{\alpha\dagger}_p(q,t), J^{\beta}_p(q,t')]\rangle_0 .$$

As we have shown, to calculate $\Pi^R_{\alpha\beta}$ in finite temperatures, one calculates

$$\Pi_{\alpha\beta}(q,z) = -\frac{1}{V}\langle T_z\, J^{\alpha\dagger}_p(q,z)\, J^{\beta}_p(q,0)\rangle \quad --- ②$$

$$\Pi_{\alpha\beta}(q,i\omega) = \int_0^\beta dz\; e^{i\omega z}\,\Pi_{\alpha\beta}(q,z)$$

and makes the following change

$$\Pi_{\alpha\beta}(q,i\omega)\Big|_{i\omega\to\omega+i\delta} \longrightarrow \Pi_{\alpha\beta}(q,\omega)$$

DC conductivity

The dc conductivity is obtained at the limit of $q\to0$ & $\omega\to0$. However, the correct limit is $q\to0$ first then $\omega\to0$. Wrong answers may be obtained if the order of limit is reversed. This is understandable as if $\omega\to0$

first, $\omega=0$, $q\neq 0$ describes a static electric field and charges will seek a new equilibrium which may not go back to the true equilibrium at $q\to 0$.

Hence one defines

$$\lim_{q\to 0} \sigma_{\alpha\beta}(q,\omega) = \sigma_{\alpha\beta}(\omega)$$

$$\& \quad \lim_{q\to 0} \Pi^R_{\alpha\beta}(q,\omega) = \Pi^R_{\alpha\beta}(\omega)$$

then $\sigma_{DC} = \lim_{\omega\to 0} \mathrm{Re}\,\sigma_{\alpha\beta}(\omega)$, Normal metal $\underline{\mathrm{Im}\,\sigma_{\alpha\beta}(\omega\to 0)=0}$

It may seem that $\omega\to 0$ is ill-defined due to the presence of $\frac{i}{\omega}$ in eq. ①.

However, since $\langle n\rangle_0$ is real, one gets

$$\mathrm{Re}\,\sigma_{\alpha\beta}(\omega) = \frac{-1}{\omega}\mathrm{Im}\left[\Pi^R_{\alpha\beta}(\omega)\right]$$

Using the Lehmann representation ($\hat{O}\equiv J^\alpha_p$) (eq. 188),

$$\Pi^R_{\alpha\beta}(\omega) = \frac{e^{\beta\Omega}}{\underset{\leftarrow q=0}{V}} \sum_{n,m} \langle n|J^{\alpha\dagger}_p|m\rangle\langle m|J^\beta_p|n\rangle \frac{e^{-\beta E_n}-e^{-\beta E_m}}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}$$

$$\therefore \frac{-\mathrm{Im}\,\Pi^R_{\alpha\beta}(\omega)}{\omega} = \frac{\pi e^{\beta\Omega}}{V}\frac{(1-e^{-\beta\omega})}{\omega}\sum_{n,m}\langle n|J^{\alpha\dagger}_p|m\rangle\langle m|J^\beta_p|n\rangle e^{-\beta E_n} \times \delta(\omega+E_n-E_m) \quad (\hbar=1)$$

It is seen that the $\omega \to 0$ is well defined:

$$\lim_{\omega\to 0} \frac{1-e^{-\beta\omega}}{\omega} = \beta$$

and
$$\mathrm{Re}\,\sigma_{\alpha\beta} = \frac{\pi\beta}{V} e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} \langle n|J_\alpha^+|m\rangle\langle m|J_\beta|n\rangle \times \delta(E_n - E_m) \quad \text{---} ③$$

Diamagnetic current

The diamagnetic current contributes $\mathrm{Im}\,\sigma_{\alpha\beta}$ and is non-dissipative.

In general, it will be cancelled by combining it with $\Pi^R_{\alpha\beta}$.

To understand it, recall the Drude formula

$$\frac{d\vec{p}}{dt} = (-e)E - \frac{\vec{p}}{\tau} \Rightarrow J_e(\omega) = n_0(-e)v(\omega)$$

$$v(\omega) = \frac{(-e)E(\omega)}{m(1/\tau - i\omega)} \quad = \frac{n_0 e^2}{m}\frac{1}{1/\tau - i\omega} E(\omega)$$

$$\therefore \sigma(\omega) = \frac{n_0e^2}{m}\frac{1}{1/\tau - i\omega} \xrightarrow[\tau\to\infty]{} -\frac{1}{i\omega}\frac{n_0e^2}{m}$$

is purely diamagnetic?? This actually corresponds to $\underline{\mathrm{Re}\,\Pi^R_{\alpha\beta}(\omega)}$!

For realistic systems, $\langle \Pi^R_{\alpha\beta}(\omega) \rangle = -\delta_{\alpha\beta}(1 + i\omega\tau + \cdots)\frac{n_0e^2}{m}$

$$\therefore \sigma_{\alpha\beta}(\omega) = \frac{n_0e^2}{m}\delta_{\alpha\beta}\left(\cancel{\frac{1}{i\omega}} + \tau\right) - \frac{1}{i\omega}n_0e^2\cancel{\delta_{\alpha\beta}} = \delta_{\alpha\beta}\frac{n_0e^2}{m}\tau!$$

That is, the system will adjust the wavefunction so that the paramagnetic current cancells the contribution of diamagnetic current!

From the symmetric point of view,

$$\vec{J}(t) = \int \sigma(t-t')\, \vec{E}(t')\, dt'$$

$\vec{J}$ is odd in t
$\vec{E}$ " even " t

$\sigma = \sigma_{odd} + \sigma_{even}$

$\therefore$ σ_{odd} conforms with $\vec{J}$ $\therefore$ it does not load change of $\vec{J}$. $\therefore$ σ_{odd} is non-dissipative

While σ_{even} does not conform with $\vec{J}$, it is dissipative.

For a normal metal, there is always dissipation. $\therefore$ $\mathrm{Im}\,\sigma_{\alpha\beta}(\omega)$ $(= \sigma_{odd}(\omega)) = 0$

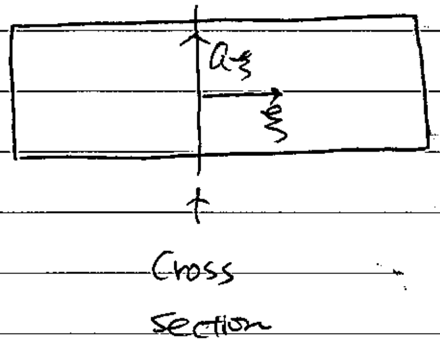
As it turns out, for superconductors, there is no dissipation, $\therefore$ $\sigma_{even} = 0$. $\mathrm{Re}\,\sigma_{\alpha\beta}(\omega) = 0$

In this case, the wavefunction is rigid so that the paramagnetic current does not cancel the contribution of the diagmetic current.

In fact, $\vec{J} = -\frac{n_s e^2}{m}\vec{A}$, which is known as the London equation!

Kubo formula for Conductance

In real experiments, the conductance is often measured. In this case, $I = G V$



I is the current across a cross section

V = voltage drop

$\therefore G = \sigma \frac{W}{L}$ W = width of circuit, L = length of circuit.

If we denote the area element in a cross section by da_ξ and coordinate perpendicular to the cross section by ξ, one has

$$I = \int da_\xi \; J_\alpha \hat{\xi}_\alpha \hookrightarrow \vec{J}\cdot\hat{\xi}$$

$$= \int da_\xi \int d\vec{r}\,' \; \hat{\xi}_\alpha \, \mathrm{Re}\,\sigma_{\alpha\beta} \; E^\beta(\vec{r}\,')$$

$\because \int d\vec{r}\,' = \int da_\xi' \int d\xi'$, for a circuit $\vec{E} = E(\xi)\hat{\xi}$, we get

$$I(\xi) = \lim_{\omega \to 0^+} \int d\xi' \; \mathrm{Re}\left[\int da_\xi \int da_\xi' \; \hat{\xi}_\alpha \, \mathrm{Re}\,\sigma_{\alpha\beta} \, \hat{\xi}'_\beta\right] E(\xi')$$

$$\equiv \int d\xi' \; G(\xi, \xi') \; E(\xi') \quad \text{--} \; ④$$

By current conservation, we arrive at

$J(\xi) = I$, $G(\xi, \xi') = G(\xi')$

$\because$ $G(\xi, \xi')$ (Kubo formula) $= G(\xi', \xi)$

$\therefore$ $G(\xi, \xi) = G$

$I = G \int d\xi' \, E(\xi') = G V$

with

$$G = \lim_{\omega \to 0^+} \mathrm{Re} \frac{-i}{\omega} C^R_{II}(\omega) = \lim_{\omega \to 0} \frac{-1}{\omega} \mathrm{Im} \, C^R_{II}(\omega)$$

$$C^R_{II}(t-t') = -i \theta(t-t') \langle [\hat{I}(t), \hat{I}(t')] \rangle \quad \cdots ⑤$$

Here we made use of $I = \int da_\xi \, J_\alpha \hat{\xi}_\alpha$ ..

Eq. ⑤ is the Kubo formula for conductance.

<u>Other Kubo formulas</u>

<u>Dielectric function</u>

The external electric field will get screened in materials. This is formulated by writing the total electric potential

$$\phi_{tot} = \phi_{ext} + \phi_{induced}$$

$$= \varepsilon^{-1} \phi_{ext} . \quad \varepsilon \equiv \text{Relative permittivity}$$

$\Rightarrow \phi_{tot}(\vec{r} t) = \int dt' \int d\vec{r}' \, \underbrace{\epsilon^{-1}(\vec{r} t, \vec{r}' t')}_{\text{dielectric function}} \phi_{ext}(\vec{r}' t')$ --- ⑥

To find Φ_{total}, one first finds Φ_{ind} through $\rho_{induced}$! This is where the Kubo formula is useful.

First, one has

$$H' = \int d^3\vec{r}'\, \rho_e(\vec{r}',t)\, \Phi^{ex}(\vec{r},t)$$

$$= \int d^3\vec{r}'\, n(\vec{r}',t)\, e\phi^{ext}(\vec{r},t) \qquad (e<0)$$

$\therefore \quad \hat{O} = \hat{n}$

$$\delta\langle n(\vec{r},t)\rangle = \int_{t_0}^{\infty} dt' \int d^3\vec{r}'\, D^R_{nn}(rt, r't')\, e\phi^{ext}(\vec{r}',t')$$

$$D^R_{nn}(rt;r't') = -i\theta(t-t')\,\langle[\hat{n}(rt), \hat{n}(r't')]\rangle_0 \qquad (\hbar = 1)$$

$$\therefore \underbrace{\delta\langle\rho_e(\vec{r},t)\rangle}_{\substack{\shortparallel \\ \rho_{ind}}} = \int_{t_0}^{\infty} dt \int d^3\vec{r}'\, D^R_{\rho\rho}(rt;r't')\, \phi_{ext}(\vec{r}',t')$$

$$D^R_{\rho\rho}(rt;r't') = -i\theta(t-t')\,\langle[\hat{\rho}_e(rt), \hat{\rho}_e(r't')]\rangle_0$$

⌞ -- ⑦

Now $\Phi_{ind}(\vec{r}) = \int d\vec{r}'\, V_c(r-r')\, \rho_{ind}(r')$ $\quad V_c = \frac{1}{|r-r'|}$

$$\therefore \Phi_{tot}(\vec{r}) = \phi_{ext}(\vec{r}) + \int d\vec{r}''\, V_c(r-r'')\, \rho_{ind}(r'',t)$$

$$= \phi_{ext}(\vec{r}) + \int d\vec{r}'' \int d\vec{r}' \int dt'\, V_c(r-r'')\, D^R_{\rho\rho}(r''t, r't')\, \phi_{ext}(r',t')$$

$$\equiv \int dt' \int dr'\, \epsilon^{-1}(rt, r't')\, \phi_{ext}(r',t')$$

eq ⑧

Hence

$$\epsilon^{-1}(\vec{r}t;\vec{r}'t') = \delta(r-r')\delta(t-t') + \int d\vec{r}''\, V_C(r-r'')\, D^R_{\rho\rho}(\vec{r}''t,\vec{r}'t') \quad \text{--- ⑧}$$

In the Fourier space, eq.⑨ becomes

$$\delta\langle\hat{\rho}(k,\omega)\rangle = D^R(k,\omega)\,\Phi_{ext}(k,\omega)$$

∴ The polarizability function (generalized susceptibility)

$$\chi^R_e(k,\omega) \equiv \left.\frac{\delta\langle\hat{\rho}_e(k,\omega)\rangle}{\Phi_{ext}(k,\omega)}\right|_{\Phi_{ext}\to 0} = D^R_{\rho\rho}(k,\omega)$$

Eq.⑧ becomes

$$\epsilon^{-1}(q,\omega) = 1 + V_c(\vec{q})\,\chi^R_e(q,\omega) \quad \text{--- ⑨}$$

$$\epsilon(q,\omega) = \frac{1}{1+V_c(q)\,\chi^R_e(q,\omega)}$$

Consider a point q at r=0.

$$\Phi_{ex} = \frac{1}{r}$$

$$\Phi_{ex}(q,\omega) = \frac{4\pi}{q^2}\,\delta(\omega) = V_c(q)\,\delta(\omega)$$

$$\Phi_{tot}(q,\omega) = \Phi_{ext}(q,\omega) + V_c(q)\,\rho_{ind}(q,\omega)$$

$$= \Phi_{ext}(q,\omega) + V_c(q)\,D^R(q,\omega)\,\Phi_{ext}(k,\omega)$$

$$= \frac{1}{\epsilon(q,\omega)}\,\Phi_{ext}(q,\omega) = \frac{4\pi}{\epsilon(q,\omega)}\,\frac{1}{q^2}\,\delta(\omega)$$

One sees that $\epsilon(q,\omega)$ replaces 1 and hence $\epsilon(q,\omega)$ is the dielectric function

(usually $q, \omega \to 0$, ϵ is called κ !)

Relation of $\epsilon(q,\omega)$ & $\sigma(q,\omega)$:

From the conservation of charges, one has

$$-i\omega\rho_e(\vec{q},\omega) + i\vec{q}\cdot\vec{J}_e(\vec{q},\omega) = 0 \quad \cdots ⑩$$

$$\left(\frac{\partial \rho_e}{\partial t} + \vec{\nabla}\cdot\vec{J}_e = 0\right)$$

$\because$ $\vec{J}_e(q,\omega) = \sigma(q,\omega)\vec{E}_{ext}(q,\omega)$ $\qquad$ $\vec{E}_{ext}(q,\omega) = -i\vec{q}\,\phi_{ext}(q,\omega)$

$$= -i\vec{q}\,\sigma(q,\omega)\,\phi_{ext}(q,\omega)$$

Substituting to eq.⑩, one gets

$$\omega\rho_e(q,\omega) = -iq^2\sigma(q,\omega)\phi_{ext}(q,\omega) \quad \cdots ⑪$$

Since $\rho_e = \delta\langle\hat{\rho}_e\rangle$ ($\rho_e^0 = 0$), we have

$$\rho_e(q,\omega) = \chi_e^R(q,\omega)\,\phi_{ext}(q,\omega) \quad \cdots ⑫$$

Eqs. ⑪ & ⑫ imply

$$\chi_e^R(q,\omega) = -i\frac{q^2}{\omega}\sigma(q,\omega)$$

Hence $\epsilon^{-1}(q,\omega) = 1 + V_c(q)\chi_e^R(q,\omega)$

$= 1 - i\frac{q^2}{\omega}\sigma(q,\omega)V_c(q)$ is related to $\sigma(q,\omega)$!

Dynamical magnetic susceptibility

Just as the electric field, one can probe the system by spatial & time dependent magnetic field $H(r,t)$.

$$\therefore\ H' = -g\mu_b \int d\vec{r}\ \vec{S}(\vec{r},t)\cdot\vec{H}(r,t)$$

where $\mu_b = \frac{|e|\hbar}{2m}$ = Bohr magneton, g = gyromagnetic ratio, $\vec{S}(\vec{r},t)$ = spin density

By using the generalized Kubo formula, one gets

$$\underset{\substack{\uparrow \\ \text{magnetization} = g\mu_b S_\alpha(r,t)}}{\delta\langle M_\alpha(r,t)\rangle} = +i\iint dr'\,dt'\ \theta(t-t')\ \langle[M_\alpha(r,t), M_\beta(r',t')]\rangle_0\ H_\beta(r',t')$$

$$\equiv \int dr' \int dt'\ \chi_{\alpha\beta}(rt, r't')\ H_\beta(r',t')$$

Where $\chi_{\alpha\beta}(rt, r't') = +i\theta(t-t')\ \langle[M_\alpha(rt), M_\beta(r't')]\rangle_0$ is the dynamical magnetic susceptibility.

Since $\vec{M} = g\mu_b\vec{S}$, what is really underlying is the dynamical spin susceptibility.

$$\chi_{\alpha\beta}(rt, r't') = -i\theta(t-t')\ \langle[S_\alpha(rt); S_\beta(r't')]\rangle_0 \quad \text{--- ⑬}$$

where a minus sign is used to be consistent with defitions of other linear response

For finite temperatures, one evaluates

$$\chi_{\alpha\beta}(q, i\omega) = \int_0^\beta d\tau \langle T_\tau S_\alpha(q,\tau) S_\beta(-q,0)\rangle e^{i\omega\tau}$$

and take the analytic continuation

$$\chi_{\alpha\beta}(q,\omega) = \chi_{\alpha\beta}(q, i\omega \Rightarrow \omega + i0^+) .$$

Usually, the system is isotropic, in that case one only needs to calculate χ_{zz}. Otherwise, it's often written as χ_{zz}, χ_{+-} with χ_{+-} being related to $\langle [S_+(r,t), S_-(r,t)]\rangle$.

For isotropic cases, $\chi_{\alpha\beta} = \chi\,\delta_{\alpha\beta}$

$S_\pm = S_x \pm i S_y$. $\chi_{+-} = \chi_{-+} = \chi_{xx} + \chi_{yy}$ $\therefore$ $\chi = \frac{1}{2}\chi_{+-} = \frac{1}{2}\chi_{-+}$

Fluctuation - dissipation theorem & two-particle Green's function

The Fluctuation - dissipation theorem is a powerful theorem in statistical physics to relate drag/friction to microscopic fluctuation.

In Condensed matter physics, the theorem provides a crucial link of experimental results to retarded Green's function. As we recall, scattering experiments (such as X-ray & neutron scatterings) measure density - density correlation.

'or spin-spin correlations'. How are these correlation functions related to the generalized susceptibilities in Kubo formula?

We shall show that they are linked by the fluctuation-dissipation (FD) theorem.

The original FD theorem stems from the Einstein relation noticed by Einstein for the motion of a Brownian particle:

$$D = \text{diffusion constant} = \frac{K_B T}{m\gamma} \quad \cdots ⑭$$

$m\gamma$ = drag coefficient.. $\frac{1}{m\gamma} = \mu$ = mobility

In the presence of a driven potential, the drift velocity v_d of Brownian particles is given by $v_d = -\mu \frac{dU}{dx}$ in steady state.

Hence when the particle's density is not uniform, the current is

$$j = -D\frac{dn}{dx} + v_d n$$
$$= -D\frac{dn}{dx} - \mu\frac{dU}{dx} n$$

When the system is in equilibrium, $j=0$, $n \propto e^{-U/K_BT}$

$$\therefore\ j \propto \frac{D}{k_BT}\frac{dU}{dx}n - \mu\frac{dU}{dx}n = 0$$

If $D = \mu k_BT = \frac{k_BT}{m\gamma}$, resulting in eq. ⑭.

Since one expects that in the long time limit,

$$\langle [X(t) - X(0)]^2 \rangle \sim 2Dt$$

for random walkers where X = position of a random walker.

$$\therefore\ D = \lim_{t\to\infty} \frac{1}{2t} \langle [X(t) - X(0)]^2 \rangle$$

$$\because\ X(t) - X(0) = \int_0^t v(t')dt'$$

$$\therefore\ D = \lim_{t\to\infty} \frac{1}{2t} \int_0^t dt_1 \int_0^t dt_2 \langle v(t_1) v(t_2) \rangle$$

$$\equiv \lim_{t\to\infty} \frac{1}{2t} \int_0^t dt_1\, f(t_1, t) = \lim_{t\to\infty} \int_0^t dt_2 \langle v(t) v(t_2) \rangle$$

where we made use of L Hospital's rule in the last equality.

Now $\lim_{t\to\infty} \int_0^t dt_2 \langle v(t) v(t_2) \rangle = \lim_{t\to\infty} \int_0^{t+t_2} dt_2 \langle v(t_2+t) v(t_2) \rangle$

Assuming $\lim_{t\to\infty} \langle v(t_0) v(t_0+t) \rangle = 0$ sufficiently fast,

One may replace $\int_0^{t+t_2}$ by $\int_0^{\infty}$ and set t to some large to. ($\int_{t+t_2}^{\infty} dt_2 \langle v(t_2+t) v(t_2) \rangle$ is sufficiently small) hence we get

$$D=\int_0^\infty \langle v(t_0)\, v(t_0+t)\rangle \, dt$$ for

some t_0. The Einstein relation can be cast into the form

$$\mu = \frac{1}{m\gamma} = \frac{D}{k_B T} = \frac{1}{k_B T}\int_0^\infty \langle v(t_0)\, v(t_0+t)\rangle \, dt$$

← - - ⑮

In other words, the mobility (i.e. dissipation related quantities) can be written as fluctuations of of velocities. Note that $\gamma k_B T = \langle \Delta M^2 \rangle$ (we derived before) can be also viewed an example similar to eq. ⑮

The precise meaning of FD theorem can be best understood by consider the stochastic equation that describes the Brownian particle

$$m\frac{dv}{dt} = -\beta v + f(t) \qquad - - - ⑯$$

where $\beta = m\gamma$ is the drag coefficient.

Eq ⑯ is also known as the Langevin equation.

Without $f(t)$, it is essentially the equation for electron's momentum in the Drude model.

$$\frac{d\vec{p}}{dt} = -\vec{P}/\tau ,$$

where $\frac{m}{\tau} = \beta = m\gamma$, $\therefore \gamma = 1/\tau$.

In the Drude model, $\vec{p}$ is atually the average momentum $\langle\vec{p}\rangle$.

For individual electron, f(t) acounts for the fluctuating force that each electron may experience. For a Brownian particle, f(t) is due to fluctuating force of collision with water molecules.

Now, the point of FD theorem is that the drag force is also due to collisions of water molecules.

Hence the drag coefficient β & f(t) in ⑯ must be related!

Indeed, if we denote

$$\langle f(t_1) f(t_2)\rangle = A\delta(t_1 - t_2)$$

and set $\langle f(t)\rangle = 0$, f is a Gaussian $\overset{}{\text{noise}}$ white noise (in Fourier space, $\langle f(\omega) f(\omega')\rangle = 2\pi A\,\delta(\omega+\omega')$. A independent of ω.)

For a given ensemble f(t), one can rigorously show the probability for v

$$P(v,t) \equiv \langle \delta(v - v(t)) \rangle_{\uparrow \text{average over } f}$$

Satisfies

$$\frac{dP}{dt} = \frac{d}{dv}\left[\frac{A}{m^2}\frac{d}{dv} + \gamma v\right] P \quad -- ⑰$$

which is known as the Fokker-Planck equation

Clearly, when $t \to \infty$, $P \to 0$, one obtains

$$\frac{d}{dv}\left[\frac{A}{2m^2}\frac{d}{dv} + \gamma v\right] P = 0$$

Hence $P = e^{-\alpha v^2}$ is a solution provided

$$\left(-\frac{A\alpha}{m^2} v + \gamma v\right) = 0 \quad \therefore \alpha = \frac{m^2\gamma}{A}$$

$\therefore$ If one requires $P(v, t \to \infty) = e^{-\frac{mv^2}{2k_BT}}$,

i.e., $\alpha = \frac{m}{2k_BT}$, we get

$$\frac{m^2\gamma}{A} = \frac{m}{2k_BT} \quad \therefore \underline{A = 2m\gamma k_BT} \quad \underline{= 2\beta k_BT} \quad -- ⑱$$

This is the FD theorem for Browian motion.

The noise correlation amplitude has to be $\underline{2\beta k_BT}$!

One can also understand eq. ⑱ by directly caculating $\langle v^2 \rangle$ and requiring $\langle \frac{1}{2} m v^2 \rangle = \frac{1}{2} k_B T$:

$$\because \quad m \frac{dv}{dt} + \beta v = f(t)$$

$$v(\omega) = \frac{f(\omega)}{\beta - m i \omega} = \frac{1}{\beta} \frac{f(\omega)}{1 - i\omega\tau} \qquad \tau = 1/\gamma$$

$\therefore \int dt\, e^{i\omega t} \langle v(t) v(0) \rangle \equiv$ Fourier transformation of vv correlation $\equiv S_{vv}(\omega)$

$$= \int \frac{d\omega'}{2\pi} \langle v(\omega) v(\omega') \rangle \qquad v(0) = \int \frac{d\omega'}{2\pi} v(\omega') e^{-i\omega' 0}$$

$$= \int \frac{d\omega'}{2\pi} \left(\frac{1}{\beta}\right)^2 \frac{1}{1 - i\omega\tau} \frac{1}{1 - i\omega'\tau} \underbrace{\langle f(\omega) f(\omega') \rangle}_{2\pi A \delta(\omega + \omega')}$$

$$= \frac{A}{\beta^2} \frac{1}{1 + (\omega\tau)^2}$$

$$\therefore \langle v(t) v(0) \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega t} \frac{A}{\beta^2} \frac{1}{1 + (\omega\tau)^2}$$

$$\langle v^2 \rangle = \int \frac{d\omega}{2\pi} \frac{A}{\beta^2} \frac{1}{1 + (\omega\tau)^2}$$

$$= \frac{A}{2\pi\beta^2} \frac{1}{\tau} \underbrace{\int d\tilde{\omega} \frac{1}{1 + \tilde{\omega}^2}}_{\overset{\|}{\frac{2\pi i}{2i}}} = \frac{A}{2\beta^2 \tau}$$

$$= \frac{k_B T}{m}$$

$$\therefore A = 2\beta^2 \tau \frac{k_B T}{m} = 2\beta^2 k_B T \frac{1}{m\gamma} = 2\beta k_B T$$

$$\because A = \int_0^\infty \langle f(t_0)\, f(t_0+t)\rangle \, dt$$

$\therefore$ One gets

$$\beta = \frac{1}{2k_BT}\int_{-\infty}^{\infty} \langle f(t_0)\, f(t_0+t)\rangle \, dt$$

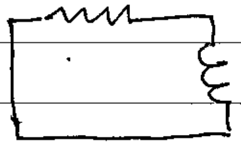
which is another manifestation of the FD theorem.

FD theorem on circuit

An application of the $\overset{\text{above}}{\frown}$ FD theorem, one

Consider a classical circuit with inductance

L & resistance R.



$$\therefore \; L\frac{dI}{dt} + RI = V \quad \text{--} ⑲$$

In the presence of capacitance, one gets

$$L\frac{{}^2d^2 q}{dt^2} + R\frac{dq}{dt} + \frac{q}{C} = V \quad \text{--} ⑳$$

In equilibrium, V = fluctuating voltage (not external voltage due to batteries).

Clearly, eq ⑲ (⑳) is the same as that for a Browian particle (eq ⑯).

$$\therefore \; R = \frac{1}{2k_BT}\int_{-\infty}^{\infty} \langle V(t_0)\, V(t_0+t)\rangle_{eq}\, dt \quad \text{-} ㉑$$

Furthermore, one expects $\langle \frac{1}{2} L I^2 \rangle = \frac{1}{2} k_B T$ is also correct.

That is, the probability of current I in a equilibrium circuit is $P(I) \propto e^{-\frac{LI^2}{2k_BT}}$

Now, for the case the voltage being dominated by R,

$$V = IR$$

Eq.② becomes $G = 1/R = \frac{1}{2k_BT} \int_{-\infty}^{\infty} \langle I(t_0) I(t_0+t) \rangle_{eq} \, dt$

L-(22)

Eq.(22) thus expresses G (conductance) as an integral of correlation function. We will come back to re-interpretate eq.(22) later.

The Fluctuation-dissipation theorem in many electron systems

We have seen the linear response function is general given by

$$G^R(t) = -i\theta(t) \langle [A(t), B(0)] \rangle \qquad \hbar \equiv 1$$

$$= -i\theta(t) \sum_n \frac{1}{Z} e^{-\beta E_n} \langle n | A(t) B(0) - B(0) A(t) | n \rangle$$

L-(23)

On the other hand, the correlation function of A & B at different time is given by

$$C_{AB}(t) = \langle A(t)\, B(0)\rangle = \sum_n \frac{1}{Z} e^{-\beta E_n} \langle n | A(t) B(0) | n\rangle$$

L. ㉔

By the Lehmann representation, we got

$$C_{AB}(\omega) = \sum_{n,m} \frac{1}{Z} e^{-\beta E_n} \langle n | A | m\rangle \langle m | B | n\rangle\, 2\pi \delta(E_n - E_m + \omega)$$

$(\hbar = 1)$

L. . . ㉕

Here at $T=0$, only $\underset{(n=0)}{E_0}$ contributes. Thus only $\omega = E_n - E_0 > 0$ contributes.

Similarly, the Lehmann representation of G^R is given by

$$G^R(\omega) = \frac{1}{Z} \sum_{n,m} \langle n | A | m\rangle \langle m | B | n\rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\omega + \hbar^{-1}(E_n - E_n) + i0^+} \quad , \cdots ㉖$$

(see eq (158) in p168)

Clearly, from eq ㉖ & ㉕, one sees that by taking $\mathrm{Im}\, G^R(\omega)$, $C_{AB}(\omega)$ & $G^R(\omega)$ can be related:

$$\therefore \mathrm{Im}\, G^R(\omega) = \frac{-\pi}{Z} \sum_{n,m} \langle n | A | m\rangle \langle m | B | n\rangle \Big(e^{-\beta E_n} - \underset{\substack{\uparrow \\ e^{-\beta E_n} e^{-\beta\omega}}}{e^{-\beta E_m}} \Big) \delta(\omega + E_n - E_m)$$

$$= -\frac{1}{2}(1 - e^{-\beta\omega}) \sum_{n,m} \frac{1}{Z} e^{-\beta E_n} \langle n | A | m\rangle \langle m | B | n\rangle\, 2\pi\delta(E_n - E_m + \omega)$$

$$\therefore \quad \mathrm{Im}\, G^R(\omega) = -\frac{1}{2}\left(1-e^{-\beta\omega}\right) C(\omega)$$

$$C(\omega) = \frac{-2}{1-e^{-\beta\omega}}\, \mathrm{Im}\, G^R(\omega)$$

$$= -2\left(1+n_B(\omega)\right) \mathrm{Im}\, G^R(\omega) \quad \cdots ㉗$$

$$n_B(\omega) = \frac{1}{e^{\beta\omega}-1}$$

Eq.㉗ is the general form of FD theorem for electronic systems. It relates the response function to the correlation function and generalizes eq.㉒ where $G = \frac{\delta I}{\delta V}$ is the linear response

$$= \frac{1}{2k_BT}\int_{-\infty}^{\infty} \langle I(t_0)\, I(t_0+t)\rangle_{eq.}\, dt.$$

Eq.㉒ can be formally derived from eq㉗ by taking the classical limit $\beta \ll 1$ $(T \to \infty)$:

$$\therefore \quad e^{-\beta\omega} \simeq 1-\beta\omega$$

$$C(\omega) = \frac{2k_BT}{\omega}\left(-\mathrm{Im}\, G^R(\omega)\right) \quad \cdots ㉘$$

Taking $\omega \to 0$ & using eq.①, one gets

$$2k_BT\, G = C(0) \quad \therefore \quad G = \frac{1}{2k_BT}\, C(0)$$

Now, $C(\omega) = \int dt\, e^{i\omega t} C(t)$

$$= \int dt\, e^{i\omega t} \langle A(t) B(0) \rangle$$

$$\therefore\ C(0) = \int_{-\infty}^{\infty} dt\, \langle A(t) B(0) \rangle$$

$$= \int_{-\infty}^{\infty} dt\, \langle A(t+t_0) B(t_0) \rangle$$

For $A = B =$ curret I, one gets

$$G = \frac{1}{2k_BT} \int_{-\infty}^{\infty} \langle I(t_0)\, I(t_0+t) \rangle_{eq.}\, dt.$$

Experimental measurements of linear response

Optical conductivity (IR) unit $1\,\mathrm{meV} = 8.0655\,\mathrm{cm}^{-1}$

($\frac{1}{\lambda}$ is the unit conventionally used)

$\sigma(\omega)$ is the typical linear response.
$(q=0)$

$50\,\mathrm{cm}^{-1} - 5\times10^{4}\,\mathrm{cm}^{-1}$
($\sim 1\,\mathrm{meV} - 1\,\mathrm{eV}$)

From $\vec{J} = \sigma(\omega)\vec{E}$

$$\vec{J} = ne\vec{v} = -i\omega ne\, X(\omega)$$

$$\therefore\ \vec{p}(\omega)\ (\text{dipole density}) = i\,\frac{\sigma(\omega)}{\omega}\,\vec{E}$$

$$\therefore\ \vec{D} = \vec{E} + 4\pi\vec{p} = \left(1 + i\,\frac{4\pi\sigma(\omega)}{\omega}\right)\vec{E} = \epsilon(\omega)\,\vec{E}$$

$$\therefore\ \epsilon(\omega) = (1 + i\,\frac{4\pi}{\omega}\,\sigma(\omega)$$

Hence measuring $\epsilon(\omega)$ effectively measures $\sigma(\omega)$.

Properties of the response function

In addition to the FD theorem, there are more useful relations.

From the Lehmann representation, one has

$$G^R_{AB}(r,r',\omega)=\frac{1}{Z}\sum_{n,m}\langle n|A(r)|m\rangle\langle m|B(r')|n\rangle\frac{e^{-\beta E_n}-e^{-\beta E_m}}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}$$

$$=\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{S(x,x',\omega')}{\omega'-\omega-i0^+}$$

$$S(x,x',\omega')=\frac{\pi}{Z}\sum_{n,m}\langle n|A(r)|m\rangle\langle m|B(r')|n\rangle\left(-e^{-\beta E_n}+e^{-\beta E_m}\right)$$

$$\times\,\delta(\omega'+\hbar^{-1}(E_n-E_m)))$$

Clearly, $\because\ \frac{1}{\omega'-\omega-i0^+}=P\frac{1}{\omega'-\omega}+i\pi\delta(\omega'-\omega)$ & $S(x,x',\omega)$ $=$ real

$$\therefore\ S(x,x',\omega)=\mathrm{Im}\,G^R_{AB}(r,r',\omega)$$

$$\therefore\ G^R_{AB}(r,r',\omega)=\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\mathrm{Im}\,G^R_{AB}(r,r',\omega)}{\omega'-\omega-i0^+}\qquad---(1')$$

Furthermore, by take complex conjugation of G^R_{AB}, one gets $\left[G^R_{AB}(r,r',\omega)\right]^*=\frac{1}{Z}\sum_{n,m}\left(\ -\ -\ \right)^*\frac{e^{-\beta E_n}-e^{-\beta E_m}}{\omega+\hbar^{-1}(E_n-E_m)-i0^+}$

exchange n & m on RHS

$$=\frac{1}{Z}\sum_{m,n}\langle m|A(r)|n\rangle^*\langle n|B(r')|m\rangle^*\frac{e^{-\beta E_m}-e^{-\beta E_n}}{+\omega+\hbar^{-1}(E_m-E_n)-i0^+}$$

$$=\frac{1}{Z}\sum_{m,n}\langle n|A^\dagger(r)|m\rangle\langle m|B^\dagger(r')|n\rangle\frac{e^{-\beta E_n}-e^{-\beta E_m}}{-\omega+\hbar^{-1}(E_n-E_m)\pm i0^+}$$

∵ $A^+ = A$, $B^+ = B$

∴ $[G^R_{AB}(r,r',\omega)]^* = G^R_{AB}(r,r',-\omega)$ - - (ii)

From (ii) ⇒ $\mathrm{Re}\, G^R_{AB}(r,r',\omega) = \mathrm{Re}\, G^R_{AB}(r,r',-\omega)$

∴ Real part of G^R_{AB} is even in ω

$\mathrm{Im}\, G^R_{AB}(r,r';-\omega) = -\mathrm{Im}\, G^R_{AB}(r,r',\omega)$

Imaginary of G^R_{AB} is odd in ω.

In addition to (i)&(ii), there are the Kramer-Kronig relations due to Causality, which will be discussed later.

For time-ordered Green's function, we have

$$G_{\alpha\beta}(rt,r't') = -i e^{\beta\Omega} \mathrm{Tr}\{e^{-\beta H} T[C_{\alpha H}(rt)\, C^{\dagger}_{\beta H}(r't')]\}$$

$$= -i\,\theta(t-t')\, e^{\beta\Omega} \sum_n e^{-\beta E_n} \langle n | C_{\alpha H}(rt)\, C^{\dagger}_{\beta H}(r't') | n \rangle$$

$$+ i\,\theta(t'-t)\, e^{\beta\Omega} \sum_n e^{-\beta E_n} \langle n | C^{\dagger}_{\beta H}(r't')\, C_{\alpha H}(rt) | n \rangle$$

$$\therefore G_{\alpha\beta}(k, t-t') = -i\,\theta(t-t')\, e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} e^{\frac{i}{\hbar}(E_n-E_m)(t-t')} (2\pi)^3 \delta(\vec{k}+\vec{P}_{nm}) \langle n | C_\alpha(0) | m \rangle \times \langle m | C^{\dagger}_\beta(0) | n \rangle$$

$$+ i\,\theta(t'-t)\, e^{\beta\Omega} \sum_{n,m} e^{-\beta E_n} e^{\frac{i}{\hbar}(E_n-E_m)(t'-t)} (2\pi)^3 \delta(\vec{k}-\vec{P}_{nm}) \times \langle n | C^{\dagger}_\beta(0) | m \rangle \langle m | C_\alpha(0) | n \rangle.$$

where $\vec{P}_{nm} = \vec{P}_n - \vec{P}_m$, $\vec{P}_n$ & $\vec{P}_m$ are the momenta of the system in states n & m.

Now, $(-i)\int_{-\infty}^{\infty} e^{i(\omega+i0^+)(t-t')} d(t-t')\ \theta(t-t')\ e^{i\hbar^{-1}(E_n-E_m)(t-t')}$

$$=(-i)\int_0^{\infty} dt\ e^{i(\omega+i0^+)t}\ e^{i\hbar^{-1}(E_n-E_m)t}$$

$$=\frac{1}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}$$

$i\int_{-\infty}^{\infty} e^{i(\omega-i0^+)(t-t')} d(t-t')\ \theta(t'-t)\ e^{i\hbar^{-1}(E_n-E_m)(t'-t)}$

$$=i\int_{-\infty}^{0} dt\ e^{i(\omega-i0^+)t-i\hbar^{-1}(E_n-E_m)t}$$

$$=\frac{1}{\omega-\hbar^{-1}(E_n-E_m)-i0^+}$$

$$\therefore G_{\alpha\beta}(K,\omega)\overset{(2\pi)^3}{=}e^{\beta\Omega}\sum_{n,m}\Big\{e^{-\beta E_n}\delta(\vec{K}+\vec{P}_{nm})\frac{\langle n|C_\alpha(\overset{r=0}{0})|m\rangle\langle m|C_\beta^{+}(0)|n\rangle}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}$$
$$+e^{-\beta E_n}\delta(\vec{K}-\vec{P}_{nm})\frac{\langle n|C_\beta^{+}(0)|m\rangle\langle m|C_\alpha(0)|n\rangle}{\omega-\hbar^{-1}(E_n-E_m)-i0^+}\Big\}$$

Exchanging n & m for the 2nd term, we get

$$G_{\alpha\beta}(K,\omega)=(2\pi)^3e^{\beta\Omega}\sum_{n,m}\delta(\vec{K}-\vec{P}_{mn})\,e^{-\beta E_n}\langle n|C_\alpha(0)|m\rangle\langle m|C_\beta^{+}(0)|n\rangle$$
$$\times\Big\{\underbrace{\frac{1}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}+e^{-\beta(E_m-E_n)}\frac{1}{\omega+\hbar^{-1}(E_n-E_m)-i0^+}}_{\parallel}\Big\}$$

$$P\frac{1}{\omega+\hbar^{-1}(E_n-E_m)}\left(1+e^{-\beta(E_m-E_n)}\right)-i\pi\delta\left(\omega+\hbar^{-1}(E_n-E_m)\right)\left(1-e^{-\beta(E_m-E_n)}\right)$$

For isotropic case, $G_{\alpha\beta} = G\,\delta_{\alpha\beta}$

$$\therefore\ G = \frac{1}{2S+1}\sum_{\alpha} G_{\alpha\alpha}$$

$$= -\frac{(2\pi)^3 e^{\beta\Omega}}{2S+1}\sum_{n,m} e^{-\beta E_n}\,\delta(\vec{k}-\vec{P}_{mn})\sum_{\alpha}|\langle n|C_\alpha(0)|m\rangle|^2$$

$$\left\{ P\frac{1}{(E_m-E_n)-\omega}\left(1+e^{-\beta(E_m-E_n)}\right)\right.$$

$$\left. +i\pi\delta(\omega-(E_m-E_n))\left(1-e^{-\beta(E_m-E_n)}\right)\right\}$$

$\therefore$ $\mathrm{Re}\,G(k,\omega)$

$$= -\frac{(2\pi)^3 e^{\beta\Omega}}{2S+1}\sum_{n,m} e^{-\beta E_n}\,\delta(\vec{k}-\vec{P}_{mn})\sum_{\alpha}|\langle n|C_\alpha(0)|m\rangle|^2$$

$$\times P\frac{1}{\omega_{mn}-\omega}\left(1+e^{-\beta\omega_{mn}}\right)$$

$$\left(\omega_{mn} = E_m - E_n\right)$$

$\mathrm{Im}\,G(k,\omega)$

$$= -\frac{(2\pi)^3 e^{\beta\Omega}}{2S+1}\sum_{n,m} e^{-\beta E_n}\,\delta(\vec{k}-\vec{P}_{mn})\sum_{\alpha}|\langle n|C_\alpha(0)|m\rangle|^2$$

$$\times \pi\delta(\omega-\omega_{mn})\left(1-e^{-\beta\omega_{mn}}\right)$$

$$\because\ \left(1+e^{-\beta\omega_{mn}}\right) = \left(1-e^{-\beta\omega_{mn}}\right)\coth\frac{\beta}{2}\omega_{mn}$$

$$\therefore\ \mathrm{Re}\,G(k,\omega) = \frac{P}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,G(k,x)}{x-\omega}\coth\frac{1}{2}\beta x\,dx \qquad \text{(Fermion)}$$

$$\mathrm{Re}\,G(k,\omega) = \frac{P}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,G(k,x)}{x-\omega}\tanh\frac{1}{2}\beta x\,dx \qquad \text{(Bosons)}$$

Now $\because\ G^R_{\alpha\beta}(rt, r't')$

$$= -i\theta(t-t')\, e^{\beta\Omega}\, \mathrm{Tr}\, e^{-\beta H}\, C_{\alpha H}(rt)\, C^\dagger_{\beta H}(r't')$$

$$-i\theta(t-t')\, e^{\beta\Omega}\, \mathrm{Tr}\, e^{\beta H}\, C^\dagger_{\beta H}(r't')\, C_{\alpha H}(rt)$$

Its Lehmann representation is

$$G^R_{\alpha\beta}(k,\omega) = (2\pi)^3 e^{\beta\Omega} \sum_{n,m} \Bigg\{ e^{-\beta E_n}\, \delta(\vec{k}+\vec{P}_{nm}) \frac{\langle n|C_\alpha(0)|m\rangle\langle m|C^\dagger_\beta(0)|n\rangle}{\omega+\hbar^{-1}(E_n-E_m)+i0^+}$$

$$+ e^{-\beta E_n}\, \delta(\vec{k}-\vec{P}_{nm}) \frac{\langle n|C^\dagger_\beta(0)|m\rangle\langle m|C_\alpha(0)|n\rangle}{\omega-\hbar^{-1}(E_n-E_m)\underbrace{+i0^+}} \Bigg\}$$

$$\therefore \begin{cases} \mathrm{Im}\, G^R(k,\omega) = -\dfrac{(2\pi)^3 e^{\beta\Omega}}{2S+1} \displaystyle\sum_{n,m} e^{-\beta E_n}\, \delta(\vec{k}-\vec{P}_{mn}) \sum_\alpha |\langle n|C_\alpha(0)|m\rangle|^2 \\ \qquad\qquad \times\, \pi\,\delta(\omega-\omega_{mn}) \underbrace{(1+e^{-\beta\hbar\omega_{nm}})}_{\begin{array}{c}\shortparallel \\ 1+e^{-\beta\omega}\end{array}} \\ \mathrm{Re}\, G^R(k,\omega) = \mathrm{Re}\, G\,(k\omega) \end{cases}$$

Compared to $\mathrm{Im}\, G(k,\omega)$, We got

$$\mathrm{Im}\, G^R(k,\omega) = \frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}}\, \mathrm{Im}\, G(k,\omega) = \coth\frac{\beta}{2}\omega\ \mathrm{Im}\, G(k,\omega)$$

$$\therefore G^R(k,\omega) = \mathrm{Re}\, G(k,\omega) + i\coth\frac{\beta\omega}{2}\, \mathrm{Im}\, G(k,\omega)$$

Similarly (Fermions)

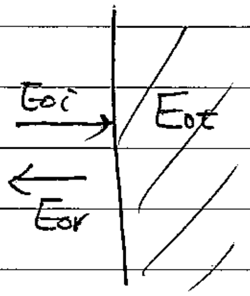
$$G^A(k,\omega) = \mathrm{Re}\, G(k,\omega) - i\coth\frac{\beta\omega}{2}\, \mathrm{Im}\, G(k,\omega)$$

For Bosons,

$$G^R(k,\omega) = \mathrm{Re}\, G(k,\omega) + i\tanh\frac{\beta\omega}{2}\, \mathrm{Im}\, G(k,\omega)$$

$$G^A(k,\omega) = \mathrm{Re}\, G(k,\omega) - i\tanh\frac{\beta\omega}{2}\, \mathrm{Im}\, G(k,\omega)$$

The complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ can be generally measured by reflectance & transimittance



$$T = \sqrt{\varepsilon_1} \left|\frac{E_{0t}}{E_{0i}}\right|^2$$

$$R = \left|\frac{E_{0r}}{E_{0i}}\right|^2$$

By solving the Maxwell eq., one finds

$$T = 1-R, \quad T = \frac{4n}{(1+n)^2+k^2}, \quad R = \frac{(1-n)^2+k^2}{(1+n)^2+k^2} \quad \text{--} ㉙$$

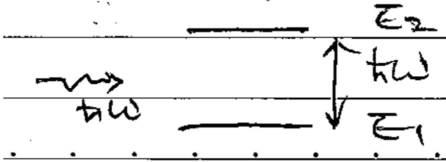
with $n = \sqrt{\dfrac{\sqrt{\varepsilon_1^2+\varepsilon_2^2}+\varepsilon_1}{2}}$ $\quad k = \sqrt{\dfrac{\sqrt{\varepsilon_1^2+\varepsilon_2^2}-\varepsilon_1}{2}}$ (exercise).

From T, one then finds ε_1 & ε_2 and thus $\sigma = \sigma_1 + i\sigma_2$ via $\varepsilon_1 = 1 - \frac{4\pi\sigma_2}{\omega}$, $\varepsilon_2 = \frac{4\pi\sigma_1}{\omega}$.

Electronic Raman scattering

The Raman scattering origins from the study of lighting scattering off atoms/molecules due to rotational/vibrational levels.

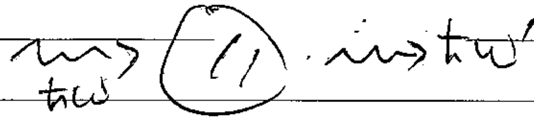
For a given two levels with E_1 + E_2



if $\hbar\omega = E_2 - E_1$, the light will be absorbed.

However, if $\hbar\omega \neq E_2 - E_1$, the light will not be absorbed and is elastically scattered!

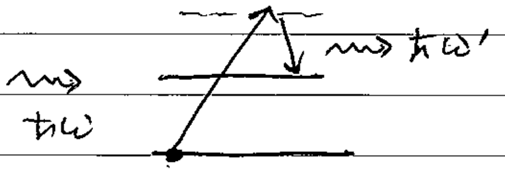
That is, $\hbar\omega = \hbar\omega'$ (scattered light). This is



the Rayleigh scattering.

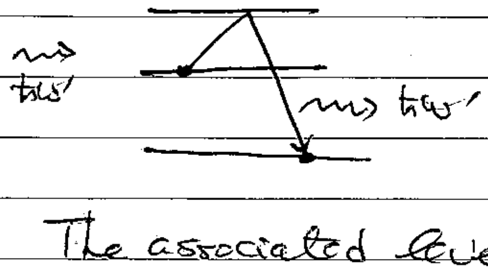
$\omega' = \omega$

Raman, however, discovered that even if $\hbar\omega \neq E_2 - E_1$, the frequency ω' of scattered light can be different from ω! This is known as Raman Scattering. Physically, it is a 2nd order effect shown in the following figures



$\hbar\omega' = \hbar\omega - \Delta E$ (Stokes line)

Fig. 1.



$\hbar\omega' = \hbar\omega + \Delta E$ (anti-Stokes line).

The associated levels on atom/molecules for Raman scatterings are originally rotation/vibrational levels.

It is later realized that electronic levels can be also involved. These are electronic Raman scatterings.

From the definition of differential cross section, since incident & outgoing photons have different frequencies, the fluxes($= \hbar k |\psi|^2$) are also different and their ratio $\propto \frac{k_s}{k_i} = \frac{\omega_s}{\omega_i}$ where i = incident and s = outgoing.

One finds

$$\frac{d^2\sigma}{d\Omega d\omega_s} = \hbar r_0^2 \frac{\omega_s}{\omega_i} R \qquad -- ⑳$$

$r_0 = e^2/mc^2$ = Thompson radius

$$R = \frac{1}{Z} \sum_{I,F} e^{-\beta E_I} |M_{FI}|^2 \delta(E_F - E_I - \hbar\Omega)$$

$\Omega = \omega_i - \omega_s$. $M_{FI} = \langle F | M | I \rangle$ = Transition amplitude. I = initial state. F = final state

Let $\vec{q} = \vec{k_i} - \vec{k_s}$ with $\vec{k_i}$ = wavenumber of incident photon & $\vec{k_s}$ = wavenumber of outgoing photon. Since effectively one electron is moved from one state to another (Fig. 1), generally by momentum conservation, electron is moved from some state with $\vec{k},\sigma$ to $\vec{k}+\vec{q},\sigma'$!

($\sigma'=\sigma$, ∵ photon doesn't couple to spin)

Hence the transition amplitude must be the form $M_{FI} = \langle F | \sum_{k\sigma} \gamma(k,q)\, C^{\dagger}_{k+q\sigma} C_{k\sigma} | I \rangle$

where $\gamma(k,q)$ is the scattering amplitude of light.

Defining a generalized density operator

$$\bar{\rho}(q) = \sum_{k\sigma} \gamma(k,q)\, C^{\dagger}_{k+q\sigma} C_{k\sigma},$$

just as the x-ray experiment, one gets

$$\frac{d^2\sigma}{d\Omega\, d\omega_s} = \hbar r_0^2 \frac{\omega_s}{\omega_i} S_{\bar{\rho}\bar{\rho}}(q,\Omega) \qquad \hbar\Omega = \hbar(\omega_i - \omega_s)$$

where $S_{\bar{\rho}\bar{\rho}}$ is $\langle \bar{\rho}\bar{\rho} \rangle$ and

$$S_{\bar{\rho}\bar{\rho}}(q,\Omega) = \int d(t-t')\, e^{i\Omega(t-t')} \langle \bar{\rho}(q,t)\, \bar{\rho}(-q,t') \rangle$$

By using the FD theorem,

$$S_{\bar{\rho}\bar{\rho}}(q,\Omega) = -2(1+n_B(\Omega))\, \mathrm{Im} \underbrace{\frac{\delta\bar{\rho}(q,\Omega)}{\delta\phi_{ext}(q,\Omega)}}_{\chi_{\bar{\rho}}(q,\Omega)}$$

$$\frac{d^2\sigma}{d\Omega d\omega_s} \propto \frac{\omega_s}{\omega_i}(1+n_B(\Omega))\,\chi''_{\bar{\rho}}(q,\Omega)$$

$(\mathrm{Im}\,\chi_{\bar{\rho}} = \chi''_{\bar{\rho}})$

Where $\chi''_{\bar{\rho}}$ is a generalized polarizability function.

When the scattering amplitude $\gamma(k,q)$ is independent of $\vec{k}, \vec{q}$. (the medium investigated is isotropic to light), γ = constant, $\bar{\rho} \propto \rho_e$ (charge density).

In this case, $\chi_{\bar{\rho}} = \chi_e^R$ (eq ⑨).

By using eq ⑨, $\mathrm{Im}\,\frac{1}{\epsilon(q,\Omega)} = \mathrm{Im}\,V_c(q)\,\chi_e^R(q,\Omega)$

$$= V_c(q)\,\mathrm{Im}\,\chi_e^R(q,\Omega)$$

$$\therefore \frac{d^2\sigma}{d\Omega d\omega_s} \propto \frac{\omega_s}{\omega_i}\,\frac{(1+n_B(\Omega))}{V_c(q)}\,\mathrm{Im}\,\frac{1}{\epsilon(q,\Omega)}$$

Hence Raman scattering measures $\mathrm{Im}\,\frac{1}{\epsilon(q,\Omega)}$
(For details, see Devereaux & Hackl Rev. Mod. Phys. 79, 175, 2007)

Magnetic neutron scattering

Similar to Raman scattering, in neutron scattering experiment, one gets

$\Omega = \omega_i - \omega_f$

$$\frac{d^2\sigma}{d\Omega d\omega_f} \propto \frac{k_f}{k_i}\sum_{\alpha\beta}(\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta)\,S^{\alpha\beta}(q,\Omega)$$

↑ ω of outgoing neutrons

where $S^{\alpha\beta}(q,\Omega) = \int d(t-t')\, e^{i\Omega(t-t')} \langle S^{\alpha}(q,t)\, S^{\beta}(-q,t')\rangle$

is the spin-spin correlation function.

From the FD theorem, one gets

$$S^{\alpha\beta}(q,\Omega) = 2(1+n_B(\Omega))\, \underbrace{\mathrm{Im}\, \chi^{\alpha\beta}(q,\Omega)}_{\text{often denoted as } \chi''(q,\Omega)} \quad \text{-- ㉛}$$

where there is no minus sign due to the minus sign in linear coupling of $\vec{H}$ to $\vec{S}$: $H' = -g\mu_b \int d\vec{r}\, \vec{S}\cdot\vec{H}$.

$\therefore\ \chi^{\alpha\beta} = +i\,\theta(t-t')\langle [S_\alpha(rt), S_\beta(r't')]\rangle$.

Note that sometimes one sees factor of 2 is replaced by $\frac{1}{\pi}$, that is due to different convention in defining $S^{\alpha\beta}(q,\Omega) = \left(\frac{1}{2\pi}\right)\int d(t-t')\, e^{i\Omega(t-t')}\langle S^{\alpha} S^{\beta}\rangle$

For isotropic cases, $\chi^{\alpha\beta} = \chi\,\delta^{\alpha\beta}$, $\chi = \frac{1}{2}\chi_{+-}$

$\therefore$ Eq. ㉛ becomes

$$S(q,\Omega) = 2(1+n_B)\,\chi'' = \frac{2\chi''(q,\Omega)}{1-e^{\beta\Omega}}$$

$$= \frac{\chi''_{+-}(q,\Omega)}{1-e^{-\beta\Omega}} \quad \text{-- ㉜}$$

Therefore, magnetic neutron scattering measures

The imaginary part of spin susceptibility.

Since the spin susceptibility is the response of spin to applied magnetic field, for ferromagnetic materials, one expects

$$\chi''(q,\Omega) \text{ peaks at } q=0, \Omega=0$$

; While for the anti ferromagnetic order,

$$\chi''(q,\Omega) \text{ peaks at } q=\overbrace{(\pi/a,\pi/a)}^{Q_{AF}}, \Omega=0$$

with $\chi(q,\Omega) = \dfrac{\Gamma_0\chi_0}{i\Omega+\Gamma_0(\xi^{-2}+(q-Q_{AF})^2)}$, ξ = correlation length.

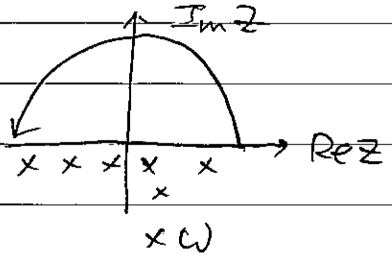
The Kramers – Kronig relation

Once $\mathrm{Im}\,\chi(q,\Omega)$ is known, one can obtain $\mathrm{Re}\,\chi(q,\Omega) \equiv \chi'(q,\Omega)$ by using the so-called Kramers-Kronig relation.

$$\mathrm{Re}\,\chi(q,\omega) = \frac{1}{\pi}\underset{\substack{\uparrow\\ \text{Cauchy principle value}}}{P}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,\chi(q,\omega')\,d\omega'}{\omega'-\omega} \quad \text{--- ㉝}$$

The Kramers – Kronig relation is a general relation applied to any response that obeys causality and is retarded!

In this case, $\chi(z)$ is analytic for $\text{Im}\, z>0$, i.e. z in the upper complex plane. All singularities of $\chi(z)$ are in the lower complex z plane.



Therefore $\oint_{\cap} \frac{\chi(z')}{z'-z}dz' = 0$ for any z in the lower complex plane.

As long as $\chi(z)\Big|_{\substack{z=Re^{i\theta} \\ R\to\infty}} \to 0$, the integral

$$\int_{\cap} \frac{\chi(z')}{z'-z}dz' \to 0 \quad \text{as} \quad R\to\infty$$

Hence $\oint_{\cap} \frac{\chi(z')}{z'-z}dz' = \int_{-\infty}^{\infty}\frac{\chi(\omega')}{\omega'-z}d\omega' = 0$ ... (34)

Now we take $z = \omega - i0^+$, ω = real, and use the fact $\frac{1}{\omega'-\omega+i0^+} = P\frac{1}{\omega'-\omega} - i\pi\delta(\omega'-\omega)$

Eq. (34) becomes $P\int_{-\infty}^{\infty}\frac{\chi(\omega')}{\omega'-\omega}d\omega' = i\pi\chi(\omega)$ -- (35)

Therefore $\text{Re}\,\chi(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\text{Im}\,\chi(\omega')\,d\omega'}{\omega'-\omega}$ (eq. (33))

$$\text{Im}\,\chi(\omega) = -\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\text{Re}\,\chi(\omega')}{\omega'-\omega}d\omega'$$

Nuclear Magnetic resonance.

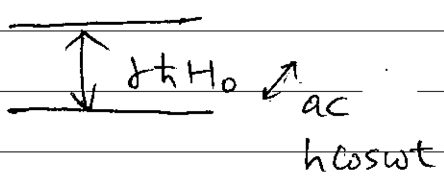
In addition to the magnetic neutron scattering, one can also probe the magnetic properties of a condensed matter system by nuclear magnetic resonance (NMR).

In this type of experiment, one applies a strong dc magnetic field $\vec{H}_0$ to align the nuclear spins $\vec{I}$.

The coupling of external field $\vec{H}_0$ & $\vec{I}$ is

$$H_{int} = -\underbrace{\gamma\hbar}_{\mu_n} \vec{I}\cdot\vec{H}_0 \quad \text{with } \gamma = \underset{\substack{\uparrow \\ \text{gyromagnetic} \\ \text{ratio}}}{g}\,\mu_n \leftarrow \text{magneton for nucleus}$$

Hence H causes Zeeman splitting.



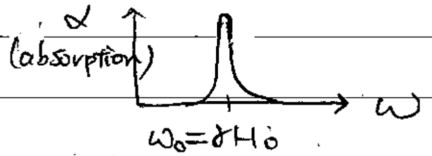
Consider two Zeeman levels for $I = \frac{1}{2}$, then $\Delta E = \gamma\hbar H_0$

One then applies a small ac field with angular frequency ω.

Clearly, when $\hbar\omega_0 = \gamma\hbar H_0$, i.e., $\omega_0 = \gamma H_0$, -- ㊱

one gets a resonance response (absorption).

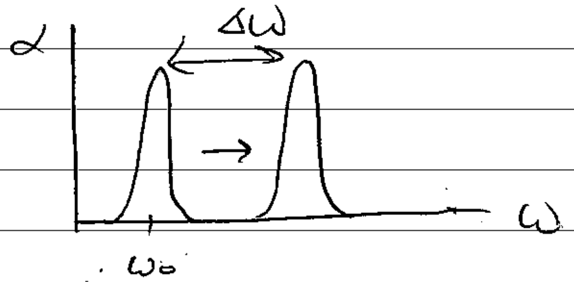
This is the <u>magnetic nuclear resonance</u>.



Knight shift

The field that acts directly on the nucleus is generally not exactly the external field H_0 as shown in eq. ㊱.

There will be correction of H_0, $\Delta\vec{H}$, due to <u>magnetization</u> of nearly electrons, which results in the shift of ω_0. Since $\vec{M} \underset{q\to0}{=} \chi(q,\omega=0)\,\vec{H}_0$, the
$q\to0$ (H_0 is uniform)
shift of ω_0 ($\Delta\omega$)



is proportional to

$$\lim_{q\to0} {}^{a}F_\alpha(q)\chi'(q,\omega=0)$$

where α denotes the direction of applied field and a indicates mass # of nucleus (such ${}^{63}Cu \rightarrow {}^{63}F_\alpha$). $F(q)$ is the form factor of spin for electron state at nucleus site

The Knight shift is defined as

$$K=\frac{\Delta\omega}{\omega_0} \quad \cdots ㊲$$

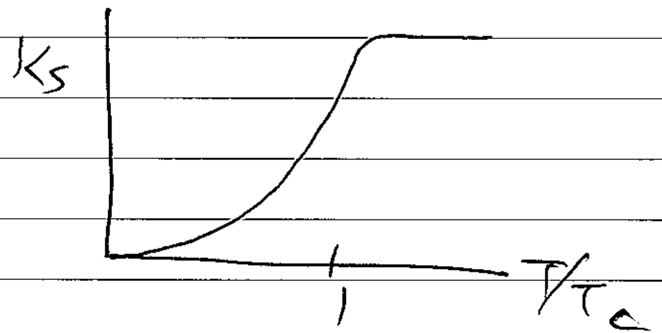
, which generally has two ↓ moreover contribution: spin & orbital of electrons

$$K = K_{spin} + K_{orb}$$

where ${}^aK_{s\alpha} \propto \lim_{q\to 0} {}^aF_\alpha(q)\,\chi'(q,\omega=0)$ .. ㊳

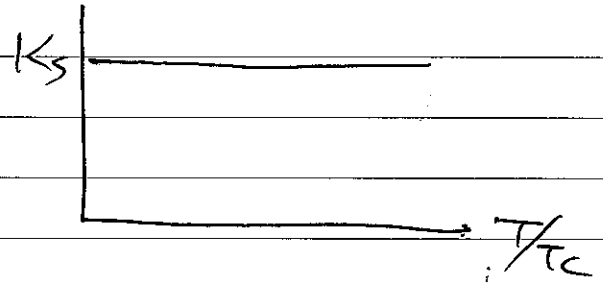
∴ Knight shift depends on magnetic polarizability of the electronic state.

For superconductors (singlet), polarizability is reduced, so that one observes



(s-wave)

Triplet pairing

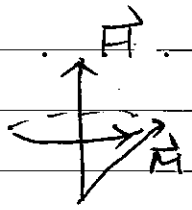


Spin-relaxation

In the presence of a field $\vec{H}$, the magnetization $\vec{M}$ ($\propto \vec{\mu}_n$) will precess

$$\frac{d\vec{\mu}_n}{dt} = \gamma\,\vec{\mu}_n \times \vec{H}$$

$$\Rightarrow \frac{d\vec{M}}{dt} = \gamma\,\vec{M} \times \vec{H}$$



When $\vec{M}$ deviates from the equilibrium value $\vec{M_0}$, it will relax back to $\vec{M_0}$

Choose $\vec{M_0} = M_0\hat{z}$, the relaxation generally obeys the Bloch equations :

$$\frac{dM_z}{dt} = \gamma(\vec{M}\times\vec{H})_z + \frac{M_0 - M_z}{T_1}$$

$$\frac{dM_x}{dt} = \gamma(\vec{M}\times\vec{H})_x - \frac{M_x}{T_2}$$

$$\frac{dM_y}{dt} = \gamma(\vec{M}\times\vec{H})_y - \frac{M_y}{T_2} \quad - \quad ㊴$$

where T_1 is termed spin-lattice relaxation time. (longitudinal)

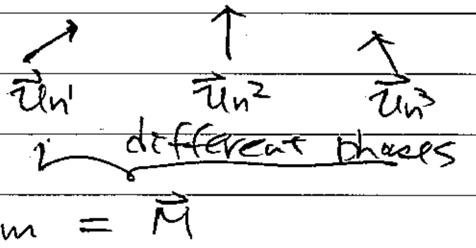
While T_2 is the transverse relaxation time or spin-spin relaxation time.

Since T_1 involves redistribution of nuclear spins to reach the thermal equilibrium, by definition, the process is not energy conservation. Furthermore, since spontaneous emission at NMR ω_0 is small, nuclear spins relax by exchanging energies with their surroundings, the lattice, allowing the spin state to change.

That is why it is called spin-lattice relaxation time. Note that when $H=0$, $M_z(t) = M_0(1-e^{-t/T_1})$.

The transverse relaxation time T_2 describes the decay of $\vec{M}_\perp$ (to $\vec{H}$). $\vec{M}_\perp = \vec{M}_\perp(0)\, e^{-t/T_2}$ (when H=0)

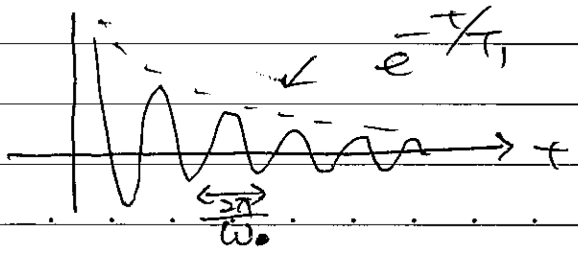
$\because$ $\vec{M}$ is the summation of $\vec{\mu}_n$. The decay of $\vec{M}_\perp$, in the microscopic picture, is due to randomization of nuclear spins $\vec{\mu}_n$.



Hence it corresponds the decoherence of nuclear spins.

Random fluctuations of local spins are the main sources for decoherence, resulting in randomize phases of different nuclear spins. Therefore, T_2 relaxation involves phases of other spins and is called "spin-spin" relaxation time.

In real experiments, one usually applies an inversion pulse and watches how the signal (absorption) oscillates and decays in time. This measures T_1



The measurement of T_2 can be done by setting $M_z=M_0$ and examining the change of M_x & M_y.

$$\frac{dM_x}{dt} = \gamma H_0 M_y - \frac{M_x}{T_2}$$

$$\frac{dM_y}{dt} = -\gamma H_0 M_x - \frac{M_y}{T_2}$$

$$\frac{dM_z}{dt} \Rightarrow$$

$\therefore$ $M_x = m e^{-t/T_2} \cos\omega t$, $M_y = -m e^{-t/T_2} \sin\omega t$

In other words, $M_x - iM_y \sim e^{i\omega t - t/T_2}$

T_2 plays the role of life time.

~~It enters into the power absorption via~~

the width : $H_x = H_1 \cos\omega t$, $H_y = -H_1 \sin\omega t$

$$P(\omega) = \frac{\omega\gamma M_z/T_2}{(\omega-\omega_0)^2 + 1/T_2^2} H_1^2 .$$

$\therefore$ The half-width of resonance at half-maximum power $\Delta\omega = 1/T_2$

$\therefore$ T_2 can be measured by width of resonance.

$\underline{1/T_1T}$: T_1 relaxation is mainly due to coupling of neuclear spin to s electrons

$H' = -\gamma\hbar \vec{I}\cdot\delta\vec{H}$; $\delta H_\pm = S_x \pm i S_y$

$\delta\vec{H}$ = fluctuating spins of electrons

$\therefore W_{b\to a} = \frac{2\pi}{\hbar} |\langle a|H'|b\rangle|^2 \delta(E_a - E_b)$ (Fermi Golden rule)
(transition rate)

where $|a\rangle = |m\rangle|\nu\rangle$ $|m\rangle$ are eigenkets to $|I_z\rangle$
$|b\rangle = |m+1\rangle|\nu'\rangle$ $|\nu\rangle$ are spin eigenstates.

$$E_a - E_b = \underbrace{E_m - E_{m+1}}_{\hbar\omega_0} + E_\nu - E_{\nu'}$$

$$\therefore \delta(E_a - E_b) = \delta(E_{\nu'} - E_\nu - \hbar\omega_0).$$

$$W_{b\to a} = \frac{2\pi}{\hbar}\left(\frac{\gamma\hbar}{2}\right)^2 |\langle m|I_+|m+1\rangle\langle\nu|\delta H_-|\nu'\rangle|^2 \delta(E_{\nu'} - E_\nu - \hbar\omega_0)$$
(transition rate) $\left(\vec{I}\cdot\delta\vec{H} = I_z\delta H_z + \frac{1}{2}I_+\delta H_- + \frac{1}{2}I_-\delta H_+\right)$

$$\because \delta(E_{\nu'} - E_\nu - \hbar\omega_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{i\left(\frac{E_{\nu'} - E_\nu}{\hbar} - \omega_0\right)t}$$

$$= \frac{\gamma^2}{2}\underbrace{[I(I+1) - m(m+1)]}_{|\langle m|I_+|m+1\rangle|^2 = (I-m)(I+m+1)}\int_{\infty}^{\infty} dt\, e^{-i\omega_0 t}\langle\nu'|e^{\frac{i}{\hbar}H_e t/\hbar}\delta H_+ e^{-\frac{i}{\hbar}H_e t} \times \delta H_-|\nu'\rangle \quad \text{--- ㊵}$$

(ν will be summed later and disappears!)

Similarly, $\frac{\gamma}{2}I_-\delta H_+$ has a similar contribution (from $a\to b$) with $\langle\nu|\delta H_-(t)\,\delta H_+(0)|\nu\rangle$ --- ㊶

$$\therefore \text{Transition rate} = \frac{1}{T_1} = \frac{\sum_{\nu,\nu'}\frac{\text{㊵}+\text{㊶}}{(I-m)(I+m+1)}e^{-\beta H_e}}{Z_e}, \text{ where}$$

the factor (I−m)(I+m+1) is the overlap of initial & final wave function of neuclear spins. and one removes it to see the transition due to the electron state.

$$\therefore \frac{1}{T_1} = \frac{\gamma^2}{2}\int_{-\infty}^{\infty} dt \cos\omega_0 t \,\langle \underbrace{\delta H_+(t)\,\delta H_-(0) + \delta H_-(t)\,\delta H_+(0)}_{\substack{\| \\ \langle S_x(t) S_x(0) + S_y(t) S_y(0)\rangle}} \rangle$$

Hence $1/T_1$ is determined by spin − spin correlation, at a particular neuclear site, say, i.
similar to neutron scattering

$$\because \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \langle S_\alpha(t) S_\alpha(0)\rangle$$

$$= \int_{-\infty}^{\infty} dt\, e^{+i\omega t} \langle \underbrace{S_\alpha(-t) S_\alpha(0)}_{\substack{\| \\ \langle S_\alpha(0) S_\alpha(t)\rangle}} \rangle$$

translationally invariant in time.

$$= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle S_\alpha(t) S_\alpha(0)\rangle$$

$$\therefore \frac{1}{T_1} = \gamma^2 \int_{-\infty}^{\infty} dt\, e^{i\omega_0 t} \langle S_x^i(t) S_x^i(0) + S_y^i(t) S_y^i(0)\rangle$$

$$= \gamma^2 \left[S_{xx}^i(\omega_0) + S_{yy}^i(\omega_0) \right]$$

In general, the neuclear spin may couple to electrons far away from site i, hence one replaces

S_α^i by $\sum_j F(i-j) S_\alpha^j$. --- ㊷ In the Fourier space,

this amounts to reploco $S_x(\omega_0)$ by $S_x(q,\omega_0) F_q$

$$\therefore \frac{1}{T_1} = \gamma^2 \sum_q F_q F_{-q} \left[S_{xx}(q,\omega_0) + S_{yy}(q,\omega_0) \right]$$

By using the FD theorem, one arrives at

$$S_{xx}(q,\omega_0) = 2(1+n_B(\Omega)) \mathrm{Im}\,\chi_{xx}(q,\omega)$$

$$\underset{\substack{\nearrow \\ \text{isotropic}}}{=} 2(1+n_B(\Omega))\chi''(q,\omega_0)$$

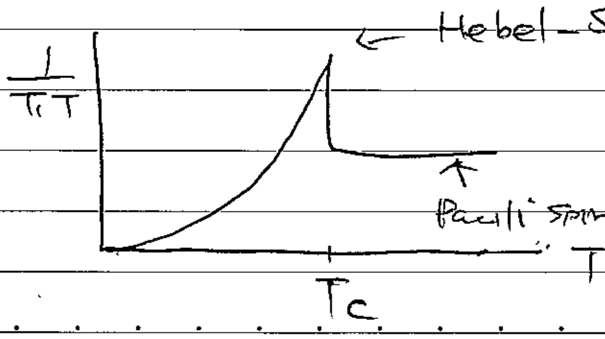
$$\therefore \frac{1}{T_1} = \gamma^2 \sum_q |F(q)|^2 \frac{4\chi''(q,\omega_0)}{1-e^{-\beta\omega_0}}$$

$$\underset{\substack{\nearrow \\ \hbar\omega_0 \ll k_B T}}{=} 4\gamma^2 k_B T \sum_q |F(q)|^2 \frac{\chi''(q,\omega_0)}{\omega_0}$$

$$= 2\gamma^2 k_B T \sum_q |F(q)|^2 \frac{\chi''_{+-}(q,\omega_0)}{\omega_0}$$

$$\therefore \frac{1}{T_1 T} \text{ measures } \sum_q |F(q)|^2 \frac{\chi''(q,\omega_0)}{\omega_0} \quad \text{-- ㊸}$$

example: BCS superconductor (singlet, rotational invariant,



$$\chi \sim \sum_q \frac{f(\xi_{k+q}) - f(\xi_q)}{\xi_{k+q} - \xi_q}$$

$$\sim \sum \frac{df}{d\xi}$$

$\frac{df}{d\xi}$ peaked at $\xi \sim \Delta_0$.

resulting in a peak at $T \lessapprox T_c$

$1/T_2$

T_2 relaxation is mainly due to interactions among neuclear spins so that each neuclear spin at each moment may experience different local field and (thus) is precessing at different angular speed, resulting in dephasing.

The coupling of nuclear spins is dominated by the one mediated by electrons:

$$H^{i} = -\gamma \frac{1}{\hbar} \sum_{j} \underbrace{\vec{I}_i \cdot F(r_i - r_j)\vec{S}_j}_{\text{acting as a local magnetic field at } j}$$

with $F(r_{ij})$ be the same form factor in eq. ㊷.

Clearly, for two nuclear spins located at i & j, their interaction can be mediated by electrons:

electrons are first polarized by $\vec{I}_i$ at r_K, the polarization extends to r_K' so that electron spin interacts with $\vec{I}_j$ at r_K'

$$\therefore\ H_{ij} = -(\gamma\hbar)^2 \sum_{r_K, r_K'} I_z(r_i)\, F(r_i, r_K)\, \chi'(r_K, r_K')\, F(r_K', r_j)\, I_z(r_j) \quad \cdots ㊹$$

Where $\chi'(r_K, r_K')$ is the static spin susceptibility and is hence the real part of $\chi(R, \omega = 0)$.

The effective coupling between $I(r_i)$ & $I(r_j)$ is

then $J_{ij} = \sum_{r r' q} \frac{-(\gamma\hbar)^2}{N} F(r_i, r') e^{iq(r'-r)} \chi'(q,0) F(r, r_j)$

For $F(r, r') = F(r-r')$, one has

$$J_{ij} = \sum_q \left[\sum_R \sum_{R'} \frac{-(\gamma\hbar)^2}{N} F(r_i - r') e^{iq(r'-r_i)} F(r-r_j) e^{iq(r_j - r)} \right]$$

$$\times e^{iq(r_i - r_j)} \frac{-(\gamma\hbar)^2}{N} \chi'(q,0)$$

$$= \frac{-(\gamma\hbar)^2}{N} \sum_q \chi'(q,0) (F(q))^2 e^{iq\cdot(r_i - r_j)}$$

Therefore, the coupling of nuclear spins is determined by J_{ij} (and thus $\chi'(q,0)$, $F^2(q)$).

By using the Fermi-Golden rule, one expects that $\frac{1}{T_2} \propto \left(\sum_q \chi'(q,0) F^2(q)\right)^2$

Hence - $1/T_2$ determines $\chi'(q,0)$.

In real experiments, however, one finds that the transition intensity profile is Gaussian-like, instead of being Lorentzian, which is the basis for the Fermi-Golden rule.

In this situation, one can approximate the effective magnetic field that acts on I_i be $\sum_j J_{ij} I_j = H_i$.

and treat H_i as a Gaussian random field.

One then expects that instead of

$$M_\perp(t) \propto e^{-t/T_2} \cos\omega_0 t$$

$$\to M_\perp(t) \propto e^{-\left(\frac{t}{T_2}\right)^2} \cos\omega_0 t$$

$$\left(\frac{1}{T_2}\right)^2 \propto \sum_{j\neq i} (J_{ij})^2$$

Standard deviation of H_i gives the suppression of $M_\perp$ and hence the width of Gaussian decay e^{-t^2/T_2^2}

(see C. Pennington & C.P. Slichter, Phys. Rev. Lett. 66, 381, 1991)

$$\because \sum_{j\neq i}(J_{ij})^2 = \sum_j (J_{ij})^2 - (J_{ii})^2$$

$$= \frac{(\gamma\hbar)^4}{N}\sum_q F^4(q)[\chi'(q,0)]^2 - \left[\frac{(\gamma\hbar)^2}{N}\sum_q F^2(q)\chi'(q,0)\right]^2$$

$$\therefore \frac{1}{T_2} \propto \frac{1}{N}\sum_q F^4(q)[\chi'(q,0)]^2 - \left(\frac{1}{N}\sum_q F^2(q)\chi'(q,0)\right)^2$$

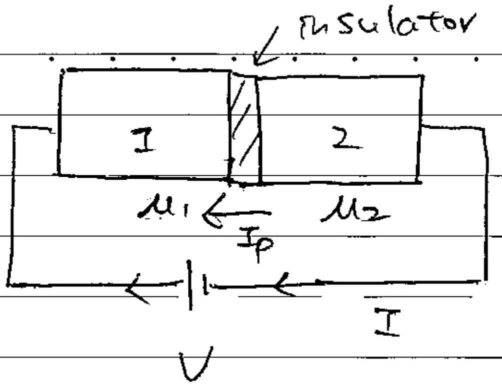
Tunneling spectroscopy.

In the above linear response, Observables involved contain two electrons. Therefore, the response functions are propagations of two electrons. We shall discuss their propagations later.

To get single-particle properties, such as one-particle, Green's function, one needs to insert/remove a single electron into/out of the many-particle system.

This can be achieved by socalled tunnel junction device or in some cases the optical measurement in which a photon couples $c^{+} c$ and photon disappears.

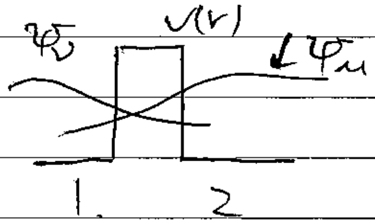
We shall examine the tunnel junction device first. In tunneling experiments two conducting materials are brought into close contact so that electrons can tunnel from one to another.



Usually, a thin insulator is placed between two materials 1 & 2. Then the system is connected to a battery forming a circuit with a current I being set up.

The whole problem can be treated as a response to the tunneling between 1 & 2.

The tunneling is induced by wave function overlaps $T_{\nu\mu}$ between two single particle particle $\underbrace{\quad\quad}_{\text{wave functions}}$ of isolated 1 and 2;



$$T_{\nu\mu} = \int dr\, \varphi_\nu^*(r)\, H(r)\, \varphi_\mu(r)$$

$$H(r) = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

Hence we can turn on the current by turning on the tunneling Hamiltonian

$$H_T = \sum_{\nu\mu} T_{\nu\mu} C_{1\nu}^\dagger C_{2\mu} + T_{\nu\mu}^* C_{2\mu}^\dagger C_{1\nu} \quad \text{---} (46)$$

Note that index μ, ν are $\vec{k}_{\parallel}$ (parallel to the tunneling junction) which are conserved during tunneling & $k_{\perp}$ (perpendicular to the junction) which are not conserved.

$\therefore$ μ & ν differ in $k_{\perp}$.

Due to the tunneling, electron numbers in 1 & 2 are no longer conserved.
(N_1) (N_2)

This results in the flow of current.

$I = -e\langle I_p \rangle$, I_p = particle current

$$I_p = \frac{dN_1}{dt} = i\,[H_T, N_1] \quad \text{where } N_1^{(t)} = e^{iH_Tt} N_1 e^{-iH_Tt}$$
$(\hbar = 1)$

$$= i \sum_{\nu\mu} \sum_{\nu'} \left[T_{\nu\mu} C_{1\nu}^{\dagger} C_{2\mu} + T_{\nu\mu}^{*} C_{2\mu}^{\dagger} C_{1\nu},\ C_{1\nu'}^{\dagger} C_{1\nu'} \right]$$

Making use of $[AB, CD]$

$$= \{A, C\} DB - C\{A, D\} B + A\{B, C\} D - AC\{B, D\},$$

We get the particle current operator

$$I_p = -i \sum_{\nu\mu} \left[T_{\nu\mu} C_{1\nu}^{\dagger} C_{2\mu} - T_{\nu\mu}^{*} C_{2\mu}^{\dagger} C_{1\nu} \right]$$

whose meaning is obvious.

Applying the Kubo formula, one turns on H_T from $t_0=-\infty$ and gets

$$\langle I_p(t)\rangle = \int_{-\infty}^{\infty} -i\Theta(t-t')\,\langle[\hat{I}_p(t), \hat{H}_T(t')]\rangle_0\, dt'$$

Let $L(t) \equiv \sum_{\nu\mu} T_{\nu\mu} C_{1\nu}^{\dagger} C_{2\mu}$, $L^{\dagger}(t) = \sum_{\nu\mu} T_{\nu\mu}^{*} C_{2\mu}^{\dagger} C_{1\nu}$

We get

$$\langle I_p(t)\rangle = -\int_{-\infty}^{t} dt' \,\langle[L(t)-L^{\dagger}(t),\ L(t')+L^{\dagger}(t')]\rangle_0 \quad \text{--}(47)$$

The average in the integrand involves two types of terms (i) $\langle L(t)L(t')\rangle_0$, $\langle L^{\dagger}(t)L^{\dagger}(t')\rangle_0$

(ii) $\langle L(t)L^{\dagger}(t')\rangle_0$, $\langle L^{\dagger}(t)L(t')\rangle_0$

$\langle L(t)L(t')\rangle_0 \sim \langle C_{1\nu}^{\dagger}C_{1\nu'}^{\dagger}C_{2\mu}C_{2\mu'}\rangle_0$ involves
$\langle L^{\dagger}(t)L^{\dagger}(t')\rangle_0 \sim \langle C_{2\mu}^{\dagger}C_{2\mu'}^{\dagger}C_{1\nu}C_{1\nu'}\rangle_0$

pair hoppings and also do not conserve particles.

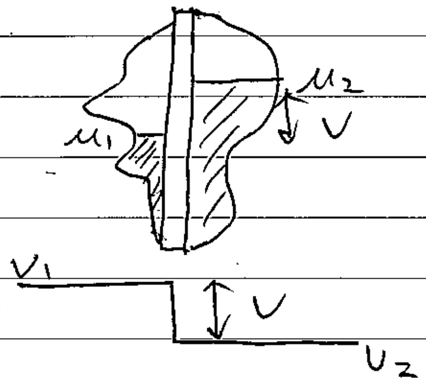
∴ They vanish for ordinary phases (except superconductors in which # of particles are not conserved.)

$$\therefore \langle I_p(t)\rangle = -\int_{-\infty}^{t} dt' \left[\langle[L(t),L^{\dagger}(t')]\rangle_0 - \langle[L^{\dagger}(t),L(t')]\rangle_0\right]$$

$$= \int_{-\infty}^{t} dt' \langle[L^{\dagger}(t),L(t')]\rangle_0 + c.c. = 2\,\mathrm{Re}\int_{-\infty}^{t} dt' \langle[L^{\dagger}(t),L(t')]\rangle_0$$

— (48)

To evaluate $\langle [L^+(t), L(t')] \rangle_0$, one notices that under the bias voltage V, if one further assumes that the voltage change occurs primarily at the junction. One can set the chemical potential of sample 1 to μ_1 and that of sample 2 to μ_2 with $\mu_2 - \mu_1 = eV > 0$



$$\mu_2 = (-e)V_2 + \mu$$
$$\mu_1 = (-e)V_1 + \mu$$

Relative to the common chemical potential at $V=0$,

One can express
$$C_1(t) = \tilde{C}_1(t)\, e^{-i\mu_1 t}$$
$$C_2(t) = \tilde{C}_2(t)\, e^{-i\mu_2 t} \quad \cdots\cdots (49),$$

From eq (49), assuming $\langle C_{1\nu} C^+_{1\nu'} \rangle \propto \delta_{\nu\nu'}$, $\langle C_{2\mu} C^+_{2\mu'} \rangle \propto \delta_{\mu\mu'}$

$$\langle I_p(t) \rangle = 2\,\mathrm{Re} \int_{-\infty}^{t} dt' \sum_{\nu\mu} \sum_{\nu'\mu'} T^*_{\nu\mu} T_{\nu'\mu'}$$
$$\langle [C^+_{2\mu}(t) C_{1\nu}(t), C^+_{1\nu'}(t') C_{2\mu'}(t')] \rangle_0$$
$$= 2\,\mathrm{Re} \int_{-\infty}^{t} dt' \sum_{\nu\mu} \sum_{\nu'\mu'} T^*_{\nu\mu} T_{\nu'\mu'} \Big(\langle C_{1\nu}(t) C^+_{1\nu'}(t') \rangle_0 \langle C^+_{2\mu}(t) C_{2\mu'}(t') \rangle_0$$
$$- \langle C^+_{1\nu'}(t') C_{1\nu}(t) \rangle_0 \langle C_{2\mu'}(t') C^+_{2\mu}(t) \rangle_0 \Big)$$
$$\underset{\substack{\nearrow \\ t \to t+t'}}{=} 2\,\mathrm{Re} \int_{-\infty}^{0} dt' \sum_{\nu\mu} |T_{\nu\mu}|^2 e^{i(\mu_1 - \mu_2)t} \big[G_1^>(\nu, -t') G_2^<(\mu, t')$$
$$- G_1^<(\nu, -t') G_2^>(\mu, t') \big] \quad \cdots (50)$$

where $G_1^{>}(\nu,-t') = -i \langle C_{1\nu}(0)\, C_{1\nu}^{+}(t') \rangle_0$, $G_2^{<}(\mu,t') = +i \langle C_{2\mu}^{+}(0)\, C_{2\mu}(t') \rangle_0$

$G_1^{<}(\nu,-t') = i \langle C_{1\nu}^{+}(t')\, C_{1\nu}(0) \rangle_0$, $G_2^{>}(\mu,t') = -i \langle C_{2\mu}(t')\, C_{2\mu}^{+}(0) \rangle_0$

are greater and lesser components we defined in the Keldysh formalism.

By going into the Fourier ω-space, one gets

$$\langle I_p \rangle = \sum_{\nu,\mu} 2\, |T_{\nu\mu}|^2\, \mathrm{Re} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \Big[G_1^{>}(\nu,\omega_1)\, G_2^{<}(\mu,\omega_2) - G_1^{<}(\nu,\omega_1)\, G_2^{>}(\mu,\omega_2) \Big]$$

$$\times \underbrace{\int_{\infty}^{0} dt'\, e^{i(-i0^+)t'}\, e^{i(\mu_1-\mu_2)t'}\, e^{i(\omega_1-\omega_2)t'}}_{\shortparallel}$$

$$\frac{-i}{\omega_1+\mu_1-\omega_2-\mu_2-i0^+} \quad \cdots (57)$$

Now, $G^{>}(\nu,t) = -i \langle C_\nu(t)\, C_\nu^{+}(0) \rangle$

$$= \frac{-i}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | C_\nu | m \rangle \langle m | C_\nu^{+} | n \rangle\, e^{\frac{i}{\hbar}(E_n-E_m)t}$$

$\therefore\ G^{>}(\nu,\omega) = \int dt\, e^{i\omega t}\, G^{>}(\nu,t)$

$$= -2\pi i \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n | C_\nu | m \rangle|^2\, \delta\big(\omega + \underset{\overset{\shortparallel}{1}}{\hbar}{}^{-1}(E_n-E_m)\big) \quad \cdots (52)$$

Similarly,

$G^{<}(\nu,t) = i \langle C_\nu^{+}(0)\, C_\nu(t) \rangle$

$$G^{<}(\nu,\omega) = 2\pi i \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n | C_\nu^{+} | m \rangle|^2\, \delta\big(\omega - \underset{\overset{\shortparallel}{1}}{\hbar}{}^{-1}(E_n-E_m)\big) \quad \cdots (53)$$

Comparing $G^<(\nu,\omega)$ & $G^>(\nu,\omega)$ with $G^R(\nu,\omega)$,

$$G^R(\nu,\omega) = \frac{1}{Z}\sum_{n,m} |\langle n|c_\nu|m\rangle|^2 \frac{e^{-\beta E_n}+e^{-\beta E_m}}{\omega+\underset{\hbar=1}{\hbar^{-1}}(E_n-E_m)+i0^+}$$

$$A(\nu,\omega) = -2\,\mathrm{Im}\,G^R(\nu,\omega)$$

$$= \frac{2\pi}{Z}\sum_{nm} |\langle n|c_\nu|m\rangle|^2 \underbrace{(e^{-\beta E_n}+e^{-\beta E_m})\,\delta(\omega+E_n-E_m)}_{\shortparallel},$$

$$e^{-\beta E_n}(1+e^{-\beta\omega})\,\delta(\omega+E_n-E_m)$$

One obtains

$$A(\nu,\omega) = i(1+e^{-\beta\omega})\,G^>(\nu,\omega)$$

$$\therefore\ iG^>(\nu,\omega) = A(\nu,\omega)\frac{1}{1+e^{-\beta\omega}} = A(\nu,\omega)(1-n_F(\omega)) \quad \cdots ㊹$$

Similarly, by exchanging n and m in eq. ㊸, one gets

$$G^<(\nu,\omega) = 2\pi i\sum_{n,m}\frac{e^{-\beta E_m}}{Z}\langle m|c_\nu^+|n\rangle\langle n|c_\nu|m\rangle\,\delta(\omega+E_n-E_m)$$

$$= 2\pi i\sum_{n,m}\frac{1}{Z}e^{-\beta(E_n+\omega)}|\langle n|c_\nu|m\rangle|^2\delta(\omega+E_n-E_m)$$

$$= -e^{-\beta\omega}G^>(\nu,\omega)$$

$$\therefore\ -iG^<(\nu,\omega) = A(\nu,\omega)\,e^{-\beta\omega}\frac{1}{(1+e^{-\beta\omega})}$$

$$= A(\nu,\omega)\,n_F(\omega) \quad \cdots ㊺$$

From eqs ㊹ & ㊺, it's clear that

$G_1^>(\nu,\omega_1)G_2^<(\mu,\omega_2) - G_1^<(\nu,\omega_1)G_2^>(\mu,\omega_2)$ is real and is given by

$$G_1^>(\nu,\omega_1)\,G_2^<(\mu,\omega_2) - G_1^<(\nu,\omega_1)\,G_2^>(\mu,\omega_2)$$

$$= A_1(\nu,\omega_1)\,A_2(\mu,\omega_2)\,(1-n_F(\omega_1))\,n_F(\omega_2)$$

$$- A_1(\nu,\omega_1)\,A_2(\mu,\omega_2)\,n_F(\omega_1)\,(1-n_F(\omega_2))$$

$$= A_1(\nu,\omega_1)\,A_2(\mu,\omega_2)\,(n_F(\omega_2)-n_F(\omega,1))$$

Hence the action of Re in ㊼ only acts on $\dfrac{-i}{\omega_1+\mu_1-\omega_2-\mu_2-i0^+} = -iP\dfrac{1}{\omega_1+\mu_1-\omega_2-\mu_2} + \pi\delta(\omega_1+\mu_1-\omega_2-\mu_2)$

$$\therefore\ \mathrm{Re}\frac{-i}{\omega_1+\mu_1-\omega_2-\mu_2-i0^+} = \pi\delta(\omega_1+\mu_1-\omega_2-\mu_2)$$

$\therefore \omega_2 = \omega_1+\mu_1-\mu_2 = \omega_1+eV$ $\therefore \omega_2$ can be integrated, we get $(\omega_1 \equiv \omega)$

$$\langle I_D\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\sum_{\mu,\nu}|T_{\nu\mu}|^2\,A_1(\nu,\omega)\,A_2(\mu,\omega+eV)$$

$$\times\,[n_F(\omega+eV)-n_F(\omega)] \quad \text{--- ㊽}$$

- If $\sum_{\mu}|T_{\nu\mu}|^2 A_2(\mu,\omega+eV) = \text{constant}$,

$$\frac{dI}{dV} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\sum_{\mu\nu}e^2|T_{\nu\mu}|^2\,A_1(\nu,\omega)\,A_2(\mu,\omega+eV)\left(-\frac{\partial n_F(\omega+eV)}{\partial\omega}\right)$$

This happens when sample 2 is choosen to be a simple metal.

$\therefore$ For $T \simeq 0$, $-\dfrac{\partial n_F(\omega+eV)}{\partial\omega} \sim \delta(\omega+eV)$,

$$\therefore \frac{dI}{dV} \propto \sum_{\nu} A_1(\nu, -eV)$$

Hence the $\frac{dI}{dV}$ versus V curve directly measures the summation of the spectral weight.

$$\sum_{\nu} A(\nu, -eV) \; !$$

In particular, for free electrons,

if $A(k,\omega)$ = bulk spectral weight

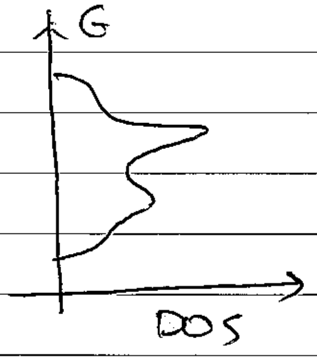
$$A(k,\omega) = -2\,\mathrm{Im}\, G^R(k,\omega) = 2\pi\,\delta(\omega - \xi_k)$$

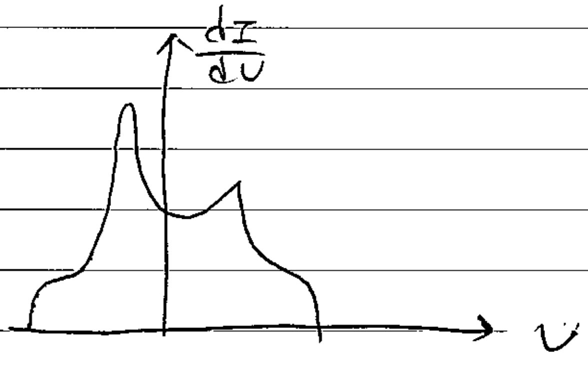
$$\therefore A(\nu,\omega) = 2\pi(\omega - \xi_\nu)$$

$$\sum_{\nu} A(\nu,\omega) \propto \text{bulk density of state}$$

$$\frac{dI}{dV} \propto \text{bulk density of state at } (-eV)$$

Example





In general, even for free electrons,

$$G^R = \sum_{\nu} \frac{\Phi_\nu^*(r)\,\Phi_\nu(r')}{\omega - \xi_\nu + i0^+}$$

$$A(\nu,\omega) = |\Phi_\nu(r)|^2 \delta(\omega-\xi_\nu)$$

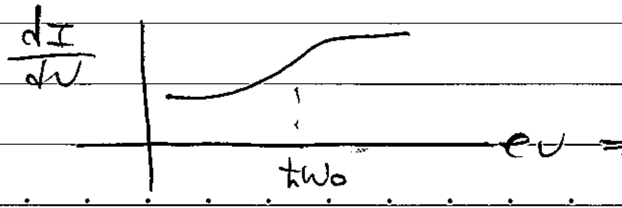
$\therefore \frac{dI}{dU} \propto \sum_\nu |\Phi_\nu(x)|^2 \delta(\omega-\xi_\nu)$ also depands on the wave function at the junction.

The above is so-called elastic tunneling spectrum in which energies of $C_{1\nu}$ & $C_{2\mu}$ only differ by the acceleration of bias voltage, i.e., eV.

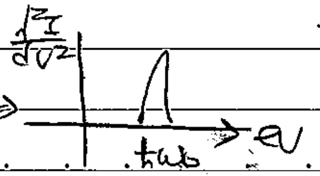
For realistic tunneling, inelastic scattering may happen. For instance, electrons can emmit phonons while they tunnel.

Since when eV hits some phonon frequency, $\hbar\omega_0$ electrons get more tunneling channel (elastic + inelastic). One expects $\frac{dI}{dU}$ increases sharply when eU goes across ... $\hbar\omega_0$.

Hence $\frac{d^2I}{dU^2}$ exhibits a peak



$\Rightarrow$



This is known as inelastic tunneling spectroscopy.

Angle resolved photoemission spectroscopy (ARPES)

Another possible way to related the linear response to single-particle Green's function is via the optical measurement. In this case, photons (EM waves) couple to electrons via the term

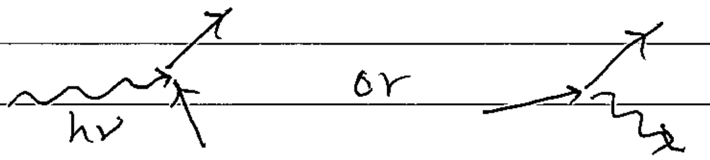
$$\vec{A} \cdot \psi^{+} \psi$$

Where in the quantum treatment, similar to the displacement field of phonons, one has

$$\vec{A} = \sum_{k\lambda} \left(\frac{2\pi}{V\omega_k}\right)^{\frac{1}{2}} \left[a_{k\lambda}\, \hat{\epsilon}(k,\lambda)\, e^{i(\vec{k}\cdot\vec{r}-\omega_k t)} + a^{+}_{k\lambda}\, \vec{\epsilon}^{*}(k,\lambda)\, e^{-i(\vec{k}\cdot\vec{r}-\omega_k t)} \right]$$

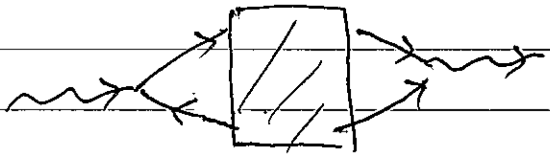
with $a_{k\lambda}$ & $a^{+}_{k\lambda}$ being creation and annihilation operators of photons.

The coupling can be represented by



(absorbing a photon). (emitting a photon)

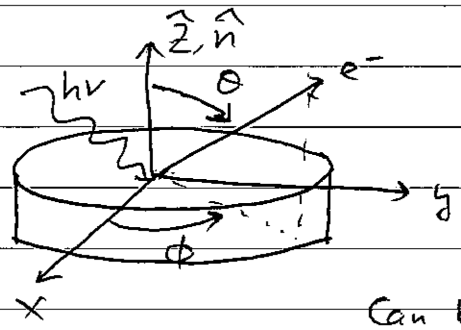
Clearly, for scattering type measurements, such as Raman scattering, x-ray scattering, photons will re-appear after interacting with materials. Two photons are involved



In this case, propagation of two electrons is involved. Hence the linear response is density-density type correlation.

To get single-particle correlation function, it is clear that only one photon line should be present and hence incident photon has to be absorbed. There are a couple of situations in which external photons (incident phtons) got absorbed such as photoemission and X-ray absorption experiments.

We shall focus on photoemission experiments. In this experiment, as shown in below,

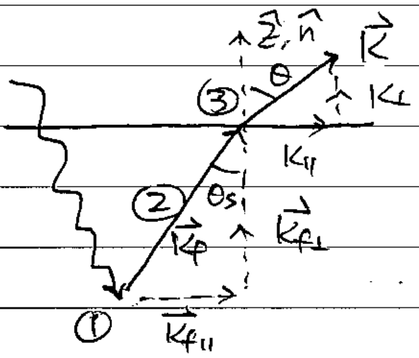


light with energy $h\nu$ illuminates the sample. Due to photoelectric effect, electrons are injected and can be collected and analyzed as a function of their energies & angles θ, ϕ.

The energy of incoming light can be varied by using sychrotron radiation source, or gas-discharge lamp.

Two typical energy range : 50eV – 2000eV (soft X-rays)
5eV – 50eV (ultra-violet regime)

Semi-classically the photoemission process can be viewed as three steps :



① intrinsic effect : optical transition of the electron between an occupied initial state and an unoccupied final state.

② Travel of photoelectron through the sample to the surface

③ Escape of electron into vacuum after transmission through the surface potential barrier.

①
In the first step, the transition takes place between the N-electron ground state Ψ_i^N with energy E_i^N and one of the possible N-electron final states Ψ_f^N of energy E_f^N, and can be

described by the Fermi's goden rule:

$$W_{if} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu)$$
$$\times \delta(\vec{k_f} - \vec{k_i} - \vec{G}) \quad \text{--} ⑤⑦$$

Whore H_{int} is the interaction Hamiltonian of the electron with the E.M. wave. and $\vec{G}$ corresponds to a reciprocal lattice vector

$$H_{int} = \frac{-e}{2mc} (\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}(r,t))$$

with $\vec{A}$ bong the vector potential for the E.M. wave.

We have chosen the gauge so that $\phi = 0$ (ϕ = scalar potential). A^2 term is dropped becaus it involves two photons. In the ultra violet regime, λ of EM waves >> atomic dimensions, $\therefore \vec{\nabla} \cdot \vec{A} \simeq 0$.

$\therefore$ One can neglect $\vec{\nabla} \cdot \vec{A}$ so that

$$H_{int} = -\frac{e}{mc} \vec{A} \cdot \vec{p} \quad \text{---} ⑤⑧$$

Near the surface, $\vec{\nabla} \cdot \vec{A} = 0$ is no longer valid. This term will nduce surface photoemission and interfere with photoemission of eq ⑤⑧ resulting in asymmetric line shapes for bulk transition peaks (see for example, T. Miller etc, PRL 77, 1167 1996).

The crucial assumption of the usual photoemission theory is to adopt the so-called <u>sudden approximation</u>. It assumes that the photo electron ϕ_f^k is instantaneously decoupled from the remaing N-1 electron after excitation & there is no interaction between the photo electron & the photo hole left. In this approximation,

$$\Psi_f^N = C_k^+ \Psi_m^{N-1} \quad \text{--} \; ⑲ \tag{59}$$

where C_k^+ is the creation operator for the photoelectron state ϕ_f^k. and Ψ_m^{N-1} is one of the energy eigenstate of N-1 electrons.

Then $$\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle = \underbrace{\langle \phi_f^k | H_{int} | \phi_i^k \rangle}_{\substack{\| \\ \text{One-particle matrix element} \\ \equiv \\ M_{fi}}} \langle \Psi_m^{N-1} | C_k | \Psi_i^N \rangle$$

$$\delta(E_f^N - E_i^N - h\nu) = \delta(\underbrace{E_{km}^{solid}} + E_m^{N-1} - E_i^N - h\nu)$$

the energy conservation implies that the difference between E_m^{N-1} and $E_i^N + h\nu$ goes to the kinetic energy of the electron in the solid

$\therefore$

$$I \propto \sum_{if} |M_{if}|^2 \sum_m |\langle \Psi_m^{N-1} | C_k | \Psi_i^N \rangle|^2 \delta(E_{km}^{solid} + E_m^{N-1} - E_i^N - h\nu) \, \delta(\vec{k}_f - \vec{k}_i - \vec{G}) \quad \text{---} \tag{60}$$

② In the 2nd step, electrons travel to the surface. In this process, they will suffer scattering and # of electrons will be limited.

The scatterings usually lead to an inelastic background on the spectrum. The wavefunction Ψ_m^{N-1}, however, is treated adiabatically without being changed.

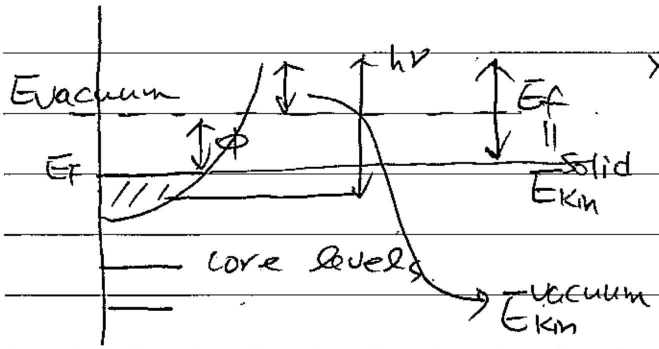
③ In the last step, electrons pass through the surface. This requires $\frac{\hbar^2}{2m}k_f^2 \geq V_0$ (surface potential barrier).

The surface potential induces a difference between the momentum paralell and perpendicular to the surface: $K_{\parallel} = k_{f\parallel} + G_{\parallel}$ is conserved, while $K_{\perp}$ is no longer conserved! Here $K_{\parallel}$ is the paralell momentum observed. For the energy, after escape to the vacuum, the electron's energy $E = E_f - \phi$ (see below)
↑ work function

Hence overal, one gets

$$I(\vec{K}, E) = \sum_{ij} |M_{fi}|^2 \sum_m |\langle \Psi_m^{N-1} | C_k | \Psi_i^N \rangle|^2$$

$$\times \delta(E_{kin}^{solid} + E_m^{N-1} - E_i^N - h\nu)\, \delta(\vec{K_f} - \vec{K_i} - \vec{G})$$



$$\times \delta(E - (E_f - \phi))\, \delta(\vec{K_{\parallel}} - \vec{k_{\parallel}} - \vec{G})$$

↑ energy of electron being detected

↑ momentum of C_k

Due to the problem of momentum non conservation in the perpendicular direction, ARPES is most powerful in probing 2D or quasi 2D materials.

In that case, $\because E(\text{detected}) = E_{kin}^{vacuum}$

$$= \frac{\hbar^2}{2m}(k_\parallel^2 + k_\perp^2)$$

$$\therefore \sqrt{2mE}\ \sin\theta = \hbar k_\parallel$$

$$I(\underset{\vec{k}_\parallel}{\underset{\equiv}{\vec{k}}},\omega) = \underbrace{I_0(\vec{k},\nu,\vec{A})}_{\propto |M_{fi}|^2} \sum_m \frac{e^{-\beta E_n}}{Z} \langle \psi_m^{N-1} | c_k | \psi_i^N \rangle$$

$$\times\ \delta(\omega + \hbar^{-1}(E_m^{N-1} - E_i^N))$$

with $\hbar\omega = E_i^N - E_m^{N-1} = E_{kin}^{solid} - h\nu$

$$= E_{kin}^{vacuum} + \phi - h\nu$$

$$= E(\text{detected}) - (h\nu - \phi)$$

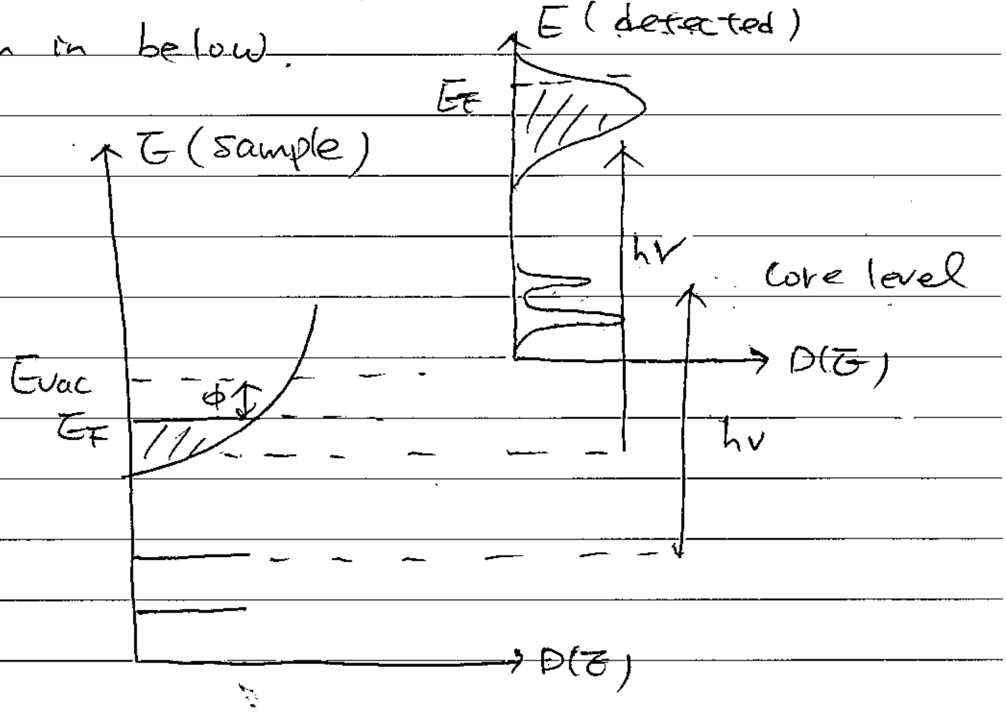
$$\because \underset{A(k,\omega)}{\underset{\parallel}{-\frac{1}{\pi} G^R(k,\omega)}} = \frac{1}{Z} \sum_{n,m} \langle n | c_k^\dagger | m \rangle \langle m | c_k | n \rangle \underbrace{(e^{-\beta E_n} + e^{-\beta E_m})}_{\substack{\parallel \\ e^{-\beta E_n}(1+e^{\beta\hbar\omega}) \\ \parallel \\ \frac{1}{n_F(\omega)}}}$$

$$\times\ \delta(\omega + \hbar^{-1}(E_m - E_n))$$

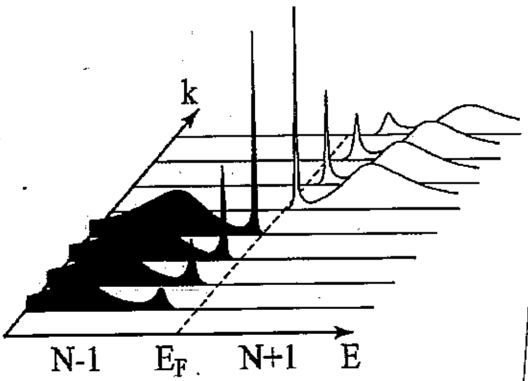
$$\therefore I(\vec{k},\omega) = I_0(\vec{k},\nu,\vec{A})\, n_F(\omega)\, A(k,\omega) \quad \text{---} ⑥①$$

∴ ARPES measures the spectral function in k & ω for 2D materials!

Due to the presence of $n_F(\omega)$, one only observes weight below the Fermi energy. See the schematic diagram shown in below.



Typical spectrum consists of a coherent peak + incoherent background :



Fermi liquid system

In real ARPES experiments, by suitable (or modeling) relation between $k_\perp$ & $k_{f\perp}$, one can get information about $k_{f\perp}$ and thus obtains spectrum for 3D materials

Two-particle Green's function and screening effect.

As we have seen, many linear responses are determined by density-density or current-current correlation functions which involve 4 Fermion operators, two creators and two annihilation operators. Hence what is involved is the two-particle Green's function.

The most typical examples are the responses of electron density & spin

$$D^R(rt;r't') = -i\theta(t-t') \langle [\hat{n}(rt), \hat{n}(r't')] \rangle_0$$

$$\chi'_{\alpha\beta}(rt;r't') = -i\theta(t-t') \langle [S_\alpha(rt), S_\beta(r't')] \rangle_0$$

Assuming H_0 is the Hamiltonian for free electrons,

$\chi_{\alpha\beta} = \chi\delta_{\alpha\beta} = \frac{1}{2}\chi_{+-}\delta_{\alpha\beta}$, $\therefore$ one needs to calculate

$$\therefore \chi_{+-}(rt;r't') = -i\theta(t-t') \langle [S_+(rt), S_-(r't')] \rangle_0$$

For translationally invariant systems, one has

$$D^R(q, t-t') = \int d(r-r')\, D^R(r-r', t-t')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}$$

$$= -i\theta(t-t') \int d(r-r')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}$$

$$\times \frac{1}{V^2} \int dq_1 \int dq_2 \langle [\hat{n}(q_1, t), \hat{n}(q_2, t')] \rangle_0$$

$$\times e^{i\vec{q}_1\cdot\vec{r}}\, e^{i\vec{q}_2\cdot\vec{r}'}$$

Clearly, if $\langle [\hat{n}(q_1,t), \hat{n}(q_2,t')] \rangle_0$

$$\equiv \tilde{D}^R(q_1, t-t')\,\delta(q_1+q_2)$$

One gets

$$\int d(r-r')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \int dq_1 \int dq_2 \,\langle [\hat{n}(q_1,t), \hat{n}(q_2,t')] \rangle_0$$

$$\times\, e^{i\vec{q}_1\cdot\vec{r}}\, e^{i\vec{q}_2\cdot\vec{r}'}$$

$$= \int dq_1 \underbrace{\int d(r-r')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}}_{V\delta(\vec{q}-\vec{q}_1)} e^{i\vec{q}_1\cdot(\vec{r}-\vec{r}')}\, \tilde{D}^R(q_1, t-t')$$

$$= V\, \tilde{D}^R(q, t-t')$$

$$\therefore\ D^R(q, t-t') = \frac{-i}{V}\theta(t-t')\, \langle [\hat{n}(q,t), \hat{n}(-q,t')] \rangle_0 \quad \text{--- (62)}$$

Similarly,

$$\chi_{+-}(q, t-t') = \frac{-i\theta(t-t')}{V} \langle [S_+(q,t), S_-(-q,t')] \rangle_0 \quad \text{--- (63)}$$

To evaluate (62) & (63), we evaluate the corresponding Motsubara Green's functions. Hence one Calculates

$$D^R(q, i\omega) = \frac{-1}{V}\int_0^\beta d(\tau-\tau')\, e^{i\omega(\tau-\tau')} \langle T_\tau\, n(q,\tau)\, n(-q,\tau') \rangle$$

($\tau-\tau'>0$ ∴ T_τ can be removed)

$$\& \ \chi_{+-}(q, i\omega) = \frac{-1}{V}\int_0^\beta d(\tau-\tau')\, e^{i\omega(\tau-\tau')} \langle T_\tau\, S_+(q,\tau)\, S_-(-q,\tau') \rangle$$

$$\because\ n(q,\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n(\tau)}\, n(i\omega_n)$$

$$\langle n(q, i\omega_n')\, n(-q, i\omega_n'') \rangle \propto \delta(\omega_n' + \omega_n'')$$

∴ τ- integral

$$\frac{1}{\beta^2}\int_0^\beta d(\tau-\tau')\, e^{i\omega(\tau-\tau')}\, e^{-i\omega_n'\tau}\, e^{i\omega_n'\tau'}$$

$$=\frac{1}{\beta}\,\delta(\omega-\omega_n')$$

$$\therefore D^R(q,i\omega_n) = \frac{-1}{\beta V}\langle n(q,i\omega_n)\, n(-q,-i\omega_n)\rangle \cdots ⑥④$$

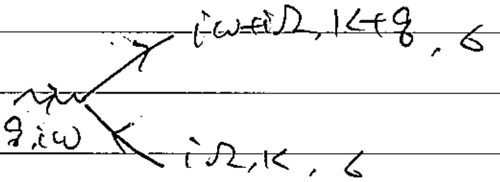
$$\chi_{+-}(q,i\omega_n) = \frac{-1}{\beta V}\langle S_+(q,i\omega_n)\, S_-(-q,-i\omega_n)\rangle \cdots ⑥⑤$$

$$\because n(q,i\omega) = \frac{1}{\beta}\sum_{\substack{k\sigma\\ i\Omega}} C^\dagger_{k+q\sigma}(i\omega+i\Omega)\, C_{k\sigma}(i\Omega)$$

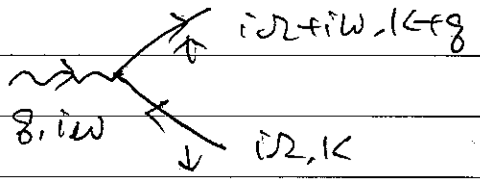
$$S_+(q,i\omega) = \frac{1}{\beta}\sum_{k\Omega} C^\dagger_{k+q\uparrow}(i\omega+i\Omega)\, C_{k\downarrow}(i\Omega)$$

$$S_-(-q,i\omega) = \frac{1}{\beta}\sum_{k\Omega} C^\dagger_{k-q\downarrow}(-i\omega+i\Omega)\, C_{k\uparrow}(i\Omega)$$

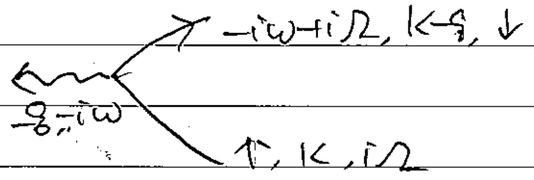
Diagramatically, $n(q,i\omega) \Rightarrow$



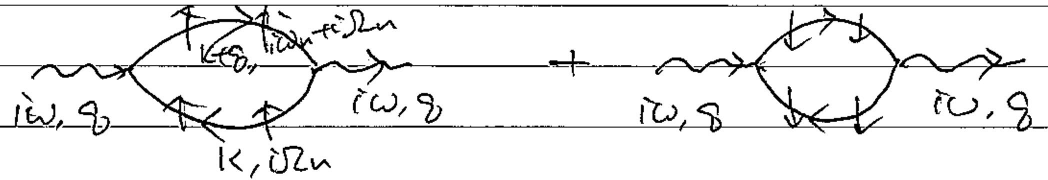
$S_+(q,i\omega) \Rightarrow$



$S_-(-q,-i\omega) \Rightarrow$



Clearly, $D^R(q,i\omega)$ can be represented by



Here the wiggle lines 〰 are introduced to represent external momentum & frequencies. Clearly, since for free electrons, G_0 is spin independent, one get,

$$D^R(q, i\omega_n) = \chi_0(q, i\omega_n) \quad \text{with}$$

$$\chi_0(q, i\omega_n) = \frac{2}{\beta V}\sum_{k,m} G_0(k, i\Omega_m)\, G_0(k+q, i\omega_n + i\Omega_m),$$

where a minus sign from the Fermion loop cancels the global minus sign.

Now, using the following frequency sum

$$\frac{1}{\beta}\sum_m \frac{1}{i\Omega_m - \xi_k}\,\frac{1}{i(\omega_n+\Omega_m) - \xi_p} = \frac{n_F(\xi_k) - n_F(\xi_p)}{i\omega_n + \xi_k - \xi_p},$$

we get

$$\chi_0(q, i\omega) = \frac{2}{V}\sum_k \frac{n_F(\xi_k) - n_F(\xi_{k+q})}{i\omega_n + \xi_k - \xi_{k+q}}$$

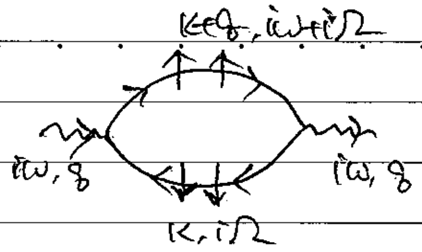
By analytic continuation, we get

$$\chi_0(q, \omega) = \frac{2}{V}\sum_k \frac{n_F(\xi_k) - n_F(\xi_{k+q})}{\omega + \xi_k - \xi_{k+q} + i0^+} \quad (66)$$

which recovers the Linhard response function we encountered when discussing CDW & SDW.

Similarly,

$\chi_{+-} =$



$||$

2χ

$$= \frac{\chi_0}{2}(q,\omega) \text{ too!} \quad \cdots \quad (66)-1$$

∴ The Linhard response function determines both the charge & spin responses.

In addition, recall that by using the local charge conservation, $\vec{J}_e(\vec{q},\omega) = \sigma(\vec{q},\omega)\vec{E}_{ext}(\vec{q},\omega)$

$$= -i\vec{q}\,\sigma(\vec{q},\omega)\,\phi_{ext}(\vec{q},\omega)$$

$$-i\omega\rho_e(\vec{q},\omega) + i\vec{q}\cdot\vec{J}_e(q,\omega) = 0$$

$$\therefore\ \omega\rho_e(q,\omega) = -iq^2\sigma(q,\omega)\,\phi_{ext}(\vec{q},\omega)$$

$$\chi_e^R(q,\omega) = -i\frac{q^2}{\omega}\sigma(q,\omega)$$

$$||$$

$$e^2 D^R(q,\omega)$$

$$\therefore\ \chi_0(q,\omega) = -i\frac{q^2}{\omega e^2}\sigma(q,\omega) ,$$

∴ $\sigma(q,\omega) = \frac{i\omega e^2\chi_0(q,\omega)}{q^2}$ is also determined by the Linhard function for free electrons.

In particular, $\text{Im}\,\chi_0(q,\omega)$ is related to $\text{Re}\,\sigma$ and corresponds to the dissipative part of conductivity.

$$-\,\mathrm{Im}\,\chi_0(\vec{q},\omega)=\frac{\pi}{V}\sum_{\vec{k}\sigma}\left(n_F(\xi_k)-n_F(\xi_{k+q})\right)\delta(\omega+\xi_k-\xi_{k+q})$$

One sees that $\mathrm{Im}\,\chi_0(-\vec{q},-\omega)=-\mathrm{Im}\,\chi_0(\vec{q},\omega)$

$$\uparrow$$

$k-q\equiv k$ (shifting k)

For isotropic systems, $\mathrm{Im}\,\chi_0(\vec{q},\omega)=\mathrm{Im}\,\chi_0(|\vec{q}|,\omega)$.

$\therefore\ \mathrm{Im}\,\chi_0(q,-\omega)=-\mathrm{Im}\,\chi_0(q,\omega)$

$\mathrm{Im}\,\chi_0(q,\omega)$ is odd in ω.

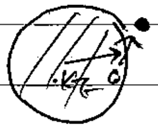
The dissipation described by is due to excitations in the systems, which is given by the δ function.

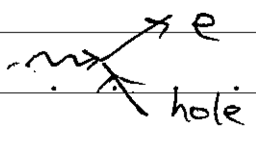
Taking $\xi_k=\frac{k^2}{2m}-\mu$ $(\hbar=1)$, the δ-function gives

$$\omega+\frac{k^2}{2m}-\frac{1}{2m}(k^2+q^2+2kq\cos\theta)=0\ \text{--}\ ⑥⑦$$

θ = angle between $\vec{k}$ & $\vec{q}$

Physically, $\hbar\omega$ is the energy of external potential (such as electric potential ~~field~~ or magnetic field). $\hbar\omega$ creates electron-hole pairs as indicated by the diagram:





Creating one electron and left a hole

$\hbar\omega$ is then the energy that can create electron-hole pair excitations. In other words, e-h pair excitations cause the dissipation.

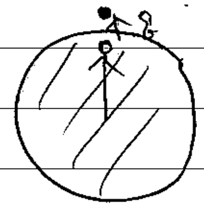
From eq. ⑥⑦, ∵ $k = 0 \to k_F$, $\cos\theta = -1 \to +1$,

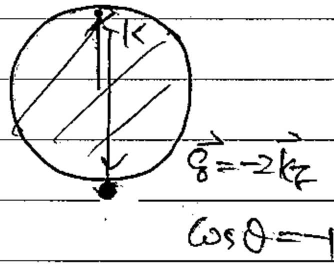
extreme values of ω are

$$\omega_{lower} = \frac{q^2}{2m} + v_F q, \quad \omega_{upper} = \frac{q^2}{2m} - v_F q$$

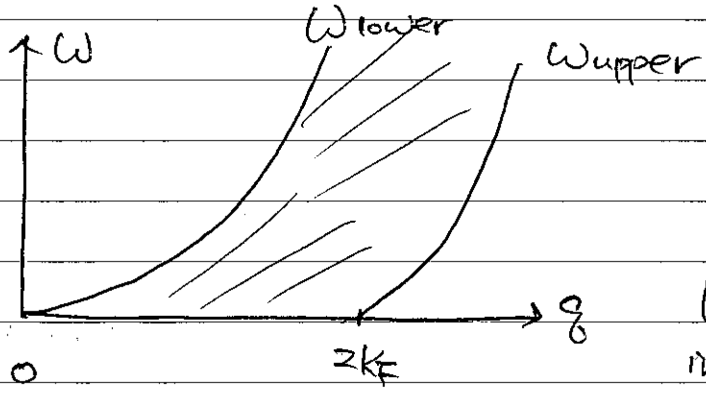
$\cos\theta = 1$ $(K = k_F, \vec{q} \to -2k_F$

$0 \le q$ $q > 2k_F)$





Hence the possible range of q and ω is given by the dashed area shown in below



Unlike simple pole excitations in single-particle Green's function there is a continuum of such excitations on two-particle Green's functions !

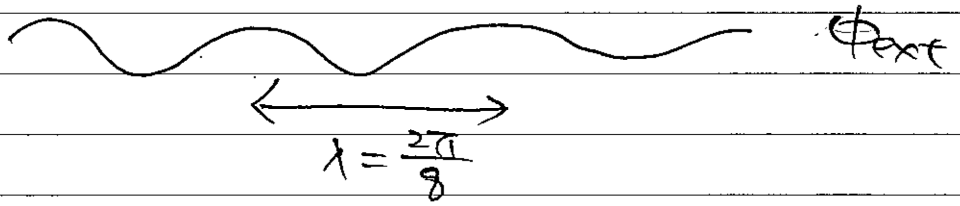
In particular, for free electrons, particle-hole excitations are the only possible source of dissipation.

Drude Conductivity & Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction

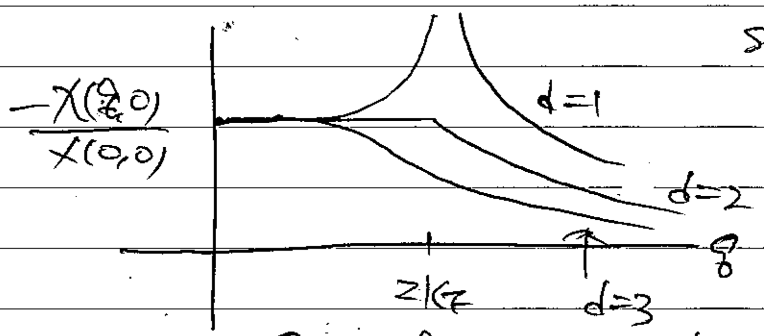
Drude conductivity : First, ∵ $\mathrm{Im}\,\chi_0(q,\omega)$ is odd in ω. ∴ $\mathrm{Im}\,\chi_0(q,0)=0$

Hence $\lim_{\omega\to 0} \mathrm{Re}\,\sigma(q,\omega) = -\frac{e^2\omega}{q^2}\,\mathrm{Im}\,\chi_0(q,\omega)\Big|_{\omega\to 0} = 0$

As we indicated earlier, this is not correct dc limit. because when $q\neq 0$, $\omega=0$, ϕ_{ext} corresponds to periodic potential and thus it can't provide current!



However, as indicated earlier, $\chi_0(q,0)=\mathrm{Re}\,\chi_0(q,0)$ may show singular behavior for d=1, 2 nested Fermi surface



Which gives rise to CDW & SDW in low dimension.

For 3D, however, we get finite $\chi_0(q,0)$

Hence $\sigma(q,0)=0$!

To get the right dc limit, one takes $q\to 0$ first.

In this case, one writes

$$\chi_0(q,\omega)=\frac{1}{V}\sum_{k\sigma}\frac{n_F(\xi_k)}{\omega+\xi_k-\xi_{k+q}+i0}-\frac{n_F(\xi_k)}{\omega+\xi_{k+q}-\xi_k+i0^+}$$

$\because \chi_0(\vec{q},\omega)=\chi_0(|\vec{q}|,\omega)$, $\therefore$ One may change ξ_{k+q} into ξ_{k+q}

$$\therefore \chi_0(q,\omega)=\frac{1}{V}\sum_{k\sigma}n_F(\xi_k)\left[\frac{1}{\omega-\omega_0+i0^+}-\frac{1}{\omega+\omega_0+i0^+}\right]$$

$$=\frac{1}{\omega+i\varepsilon}\frac{1}{V}\sum_{k\sigma}n_F(\xi_k)\left[\frac{1}{1-\frac{\omega_0}{\omega+i\varepsilon}}-\frac{1}{1+\frac{\omega_0}{\omega+i\varepsilon}}\right]$$

$$=\frac{1}{(\omega+i\varepsilon)^2}\frac{1}{V}\sum_{k\sigma}n_F(\xi_k)\,2\omega_0+O\left(\frac{\omega_0^2}{\omega^2}\right)$$

$$=\frac{1}{(\omega+i\varepsilon)^2}\underbrace{\frac{1}{V}\sum_{k\sigma}n_F(\xi_k)}_{n}\frac{1}{m}(q^2+\underbrace{\cancel{2kq\cos\theta}}_{\substack{0\\ \int d\theta\sin\theta}})$$

$$\therefore \chi_0(q\to 0,\omega)=\frac{nq^2}{m}\frac{1}{(\omega+i\varepsilon)^2}$$

Now, $\because \frac{1}{\omega+i\varepsilon}=P\left(\frac{1}{\omega}\right)-i\pi\delta(\omega)$

$$\therefore \frac{1}{(\omega+i\varepsilon)^2}=\frac{1}{\omega}P\left(\frac{1}{\omega}\right)-i\frac{\pi}{\omega}\delta(\omega)=\frac{1}{\omega^2}-\frac{i\pi}{\omega}\delta(\omega)$$

Detailed checking: $\frac{1}{(\omega+i\varepsilon)^2} = \frac{1}{(\omega^2+\varepsilon^2)^2}(\omega^2-\varepsilon^2-2i\varepsilon\omega)$

$\int_{-\infty}^{\infty} d\omega \frac{\varepsilon\omega^2}{(\omega^2+\varepsilon^2)^2} = \pi/2$, ∴ $\lim_{\varepsilon\to 0} \frac{\varepsilon\omega^2}{(\omega^2+\varepsilon^2)^2} = \frac{\pi}{2}\delta(\omega)$

$$\lim_{\varepsilon\to 0} \frac{\varepsilon\omega}{(\omega^2+\varepsilon^2)^2} = \frac{\pi}{2\omega}\delta(\omega)$$

$$\frac{1}{(\omega+i\varepsilon)^2} \to \frac{1}{\omega^2} - i\frac{\pi}{\omega}\delta(\omega)$$

∴ $\sigma(q,\omega) = \frac{ie^2\omega}{q^2}\chi_0(q,\omega) = \frac{ne^2}{m}\pi\delta(\omega) - \frac{ne^2}{im\omega}$ — (6f)

This is the conductivity for free electrons. One sees that there is a δ-peak in $\mathrm{Re}\,\sigma$ & $\mathrm{Im}\,\sigma$ (non-dissipative part) $= \frac{ne^2}{m\omega}$ does not vanishing, representing a perfect metal!

Eq. (6f) should be in contrast to predictions based on the Drude conductivity:

$$\sigma_0(\omega) = \frac{ne^2}{m}\frac{1}{1/\tau - i\omega} = \frac{ne^2}{m}\frac{1/\tau}{\omega^2+(1/\tau)^2} + i\frac{ne^2}{m}\frac{\omega}{\omega^2+(1/\tau)^2}$$

One sees that by taking $1/\tau \to 0$, one recovers eq. (6f). However, for realistic metals, τ is finite. Hence the diamagnetic (non-dissipative part) current always vanishes in the dc limit

$$\frac{ne^2}{m}\frac{\omega}{\omega^2+(1/\tau)^2} \to 0 \text{ as } \omega\to 0$$

Furthermore, the dissipative part of σ_D does not vanish as $\omega \to 0^+$, which is different from eq. (68).

Therefore, it is clear that to get the response of a perfect metal, care must be taken for the dc limit.

The correct limit for obtaing the behavior of a perfect metal is

$$q \to 0 \text{ first, then } 1/\tau \to 0, \ \omega \to 0 \text{ later.}$$

RKKY interaction

Suppose that one introduces an impurity spin $\vec{S}_j$, it would induce spin density in electron gas near $r = r_j$. The induced polarization will spread out so that another impurity spin $\vec{S}_i$ would feel it. This results in an effective coupling between $\vec{S}_i$ and $\vec{S}_j$. The coupling J_{ij} for free electron gas is known as the RKKY interaction

The coupling for impurity spins & electron gas is generally given by $H = -J \vec{S}_i \cdot \vec{S}_e(r_i) - J \vec{S}_j \cdot \vec{S}_e(r_j)$, Where $\vec{S}_c(r)$ is the spin density due to free electrons at r.

For the coupling between $\vec{S}_c$ & $\vec{S}_j$, we may consider $J\vec{S}_j$ acting as a local magnetic field to polarize $\vec{S}_c(\vec{r})$. The induced polarization $\delta\vec{S}_c$ at $\vec{r}_i$ is given by

$$\delta\langle S_c^\alpha(r_i)\rangle = \frac{\partial S_i^{c\alpha}}{\partial(JS_j^\beta)} J S_j^\beta$$

$$\xrightarrow{g\mu_b=1} = \int dt' \, i\theta(t-t') \langle[S_c^\alpha(r_i t), S_c^\beta(r_j, t')]\rangle_0 \, J S_j^\beta$$

$$= -\int dt' J\chi_{\alpha\beta}(r_i t, r_j t') S_j^\beta$$

The induced polarization changes the average of H by $H_{int} = -J\vec{S}_i\cdot\delta\vec{S}_c(r_i)\rangle$

$$= J^2 S_i^\alpha \chi_{\alpha\beta}(r_i, r_j, \omega=0) S_j^\beta$$

$$= J^2 \chi(r_i, r_j, \omega=0)\, \vec{S}_i\cdot\vec{S}_j$$

$$\therefore J_{ij} = J^2\chi(r_i, r_j, \omega=0)$$

$$\xrightarrow{\text{free electrons eq.(66)-1}} = \frac{J^2}{4}\chi_0(r_i, r_j, \omega=0) = \frac{J^2}{4}\int\frac{d^3k_1}{(2\pi)^3}\int\frac{d^3k_2}{(2\pi)^3} e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{r}} \times \frac{n_F(\vec{k}_1)-n_F(\vec{k}_2)}{k_1^2-k_2^2+i0^+}\frac{2m}{\hbar^2}$$

with $\vec{r} = \vec{r}_i - \vec{r}_j$

L84

Now, $\int \frac{d^3\vec{k}_2}{(2\pi)^3} \frac{e^{i\vec{k}_2\cdot\vec{r}}}{k_1^2-k_2^2+i0^+}$ is the Green's function

of $(E-\nabla^2)G=\delta(\vec{r})$ $E\equiv k_1^2$ for

scattering problem.

$$\therefore \int \frac{d^3\vec{k}_2}{(2\pi)^3} \frac{e^{i\vec{k}_2\cdot\vec{r}}}{k_1^2-k_2^2+i0^+} = \frac{e^{ik_1 r}}{4\pi r}$$

Similarly $\int \frac{d^3\vec{k}_1}{(2\pi)^3} \frac{-e^{-i\vec{k}_1\cdot\vec{r}}}{k_1^2-k_2^2+i0^+} = \left(\int \frac{d^3k_1}{(2\pi)^3} \frac{-e^{i\vec{k}_1\cdot\vec{r}}}{k_1^2-k_2^2-i0^+}\right)^*$

$$= \left(\int \frac{d^3k_1}{(2\pi)^3} \frac{e^{i\vec{k}_1\cdot\vec{r}}}{k_2^2-k_1^2+i0^+}\right)^* = \frac{e^{-ik_2 r}}{4\pi r}$$

$\therefore \chi_0(r, \omega=0)$

$$= \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{e^{ikr}}{4\pi r} e^{-i\vec{k}\cdot\vec{r}} + c.c.\right) \times \frac{2m}{\hbar^2}$$

$$= \frac{2\pi}{\hbar^2} \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \frac{\cos kr}{2\pi r} e^{i\vec{k}\cdot\vec{r}} \quad (\vec{k}\to-\vec{k})$$

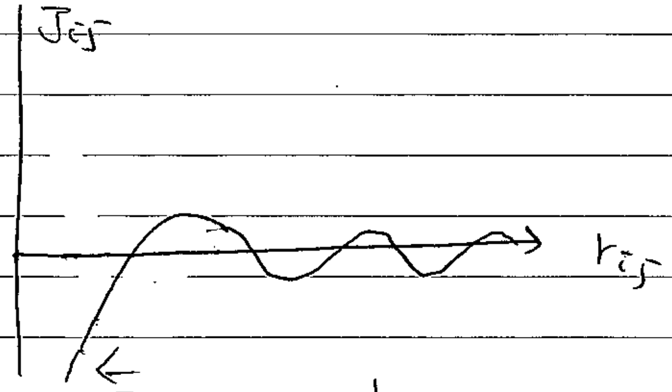
$$\because \int_0^{\pi}\int_0^{2\pi} e^{i\vec{k}\cdot\vec{r}} \sin\theta\, d\theta\, d\phi = \frac{4\pi}{kr}\sin kr$$

$$\therefore \chi_0(r,\omega=0) = \frac{1}{(2\pi)^3}\frac{2m}{\hbar^2}\frac{1}{r^2}\int_0^{k_F} k^{\cancel{2}}dk\, \frac{2\cos kr \sin kr}{\cancel{k}}$$

$$\underset{\nearrow}{=} \frac{1}{(2\pi)^3}\frac{2m}{\hbar^2}\frac{1}{r^4}\frac{1}{4}\int_0^{x} du\, u\sin u = \frac{8m}{\hbar^2(2\pi)^3} k_F^4 \frac{x\cos x - \sin x}{x^4}$$

$u=2kr$ $x=2k_F r$ L-⑥⑨

$$\therefore J_{ij} = \frac{2m}{\hbar^2}\frac{k_F^4}{(2\pi)^3}\frac{\overbrace{x_{ij}\cos x_{ij} - \sin x_{ij}}^{F(x_{ij})}}{x_{ij}^4} \qquad x_{ij} = 2k_F r_{ij}$$



$$F(x_{ij}) \to -\frac{1}{6x_{ij}} \quad x_{ij} \to 0$$

Ferromagnetic !

Random phase approximation & screening (RPA)

The density response function for free electrons $D^R = \chi_0$ is only the lowest order term for real electronic systems in which there are Coulomb interactions among electrons.

In general, one defines the time-ordered Green's function

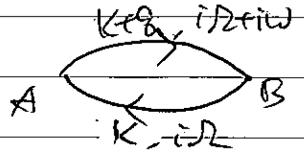
$$i D(rt, r't') = \overset{e^{\beta\Omega}}{\overset{\shortparallel}{\frac{1}{Z}}} \mathrm{Tr}\{e^{-\beta H} T[n_H(rt) n_H(r't')]\}$$

with D^R being the corresponding retarded response function.

$$D^R(rt, r't') = -i\theta(t-t') e^{\beta\Omega} \mathrm{Tr}\, e^{-\beta H} [n_H(rt), n_H(r't')].$$

In the presence of electron-electron interaction.

$V_0(q,\omega) = \frac{4\pi e^2}{q^2}\delta(\omega)$, $D_0^R = \chi_0$ is the unperturbed Green's function, represented by a bubble



. The physical picture of this diagram is <u>electron-hole pair propagation</u>: an electron is excited to above ε_F and a hole is left in the Fermi sea.

This can be also viewed as an electron and a hole are created at A and propagates to B.

Mathematically, $\chi_0(q,\tau) = -\sum_\sigma \int \frac{d^3k}{(2\pi)^3} \langle C_{k\sigma}(\tau) C^+_{k\sigma}\rangle_0$
$\langle C^+_{k+q\sigma}(\tau) C_{k+q\sigma}\rangle_0$

$C^+_{k\sigma}$ creates one electron at $\tau=0$ L-⑦⓪

Let $d^+_k \equiv C_k$, $C_{k+q\sigma} = d^+_{k+q\sigma}$ creates one hole

hole at $\tau=0$ they both vanish at τ.

In addition, D also determines the energy associated with electron-electron interaction energy: $\langle \hat{V} \rangle = \frac{1}{2}\int d^3\vec{r} \int d^3\vec{r}\,' V(\vec{r}-\vec{r}\,') \langle C^+_\alpha(r) C^+_\beta(r') C_\beta(r') C_\alpha(\vec{r})\rangle$

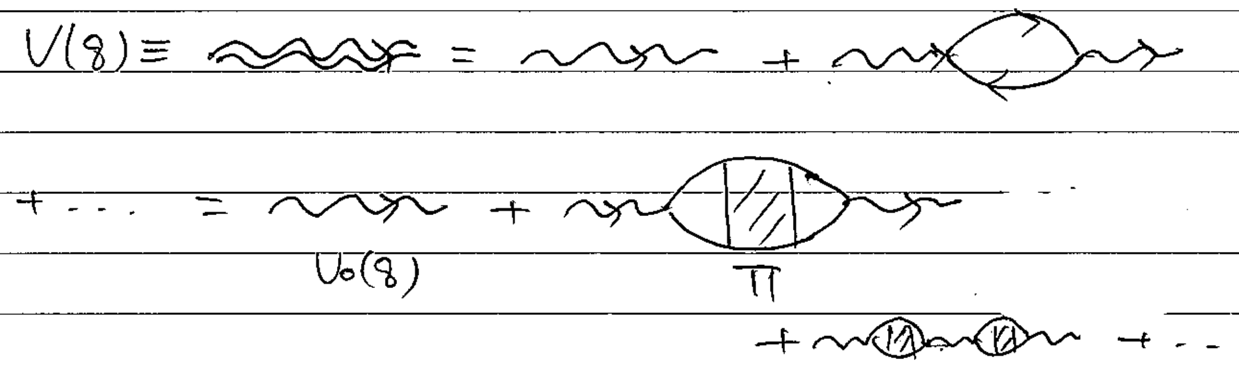
$$= \frac{1}{2}\int d^3\vec{r} \int d^3\vec{r}\,' V(\vec{r}-\vec{r}\,') \left[\langle n(\vec{r}) n(\vec{r}\,')\rangle - \delta(r-r')\langle n(r)\rangle \right]$$

where $\langle n(rt)\, n(r't) \rangle$

$= iD(rt, r', t^+)$.

The effective interaction between particles are also related to D.

Diagramatically, one has



$$\therefore\ V(q,\omega) = V_0(q,\omega) + V_0(q,\omega)\,\Pi(q,\omega)\,U_0(q,\omega) + \ldots$$

$$= V_0(q,\omega) + V_0(q,\omega)\,\Pi(q,\omega)\;V(q,\omega)$$

has absorbed (−) from V_0

"one-interaction irreducible"

$$\therefore\ V(q,\omega) = \frac{V_0(q,\omega)}{1 - V_0(q,\omega)\,\Pi(q,\omega)} \equiv \frac{1}{\epsilon(q,\omega)}\,V_0(q,\omega) \;-\; \textcircled{\Pi}$$

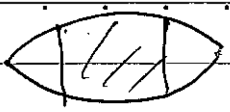
$$\epsilon(q,\omega) = 1 - V_0\,\Pi(q,\omega)$$

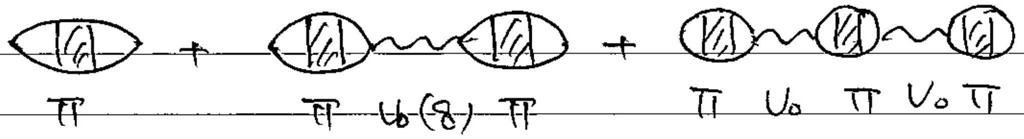
In the case of $V_0(q,\omega) = \frac{4\pi e^2}{q^2}\,\delta(\omega)$, one gets

$$V(q,\omega) = V(q)\,\delta(\omega)$$

$$V(q) = V_0(q) + V_0(q)\,\Pi(q,0)\,V(q)$$

$$V(q) = \frac{V_0(q)}{1 - V_0(q)\,\Pi(q)}$$

$D(q,\omega) =$ 

$=$ 

$+ \cdots$

$$= \Pi(q,\omega) + \Pi(q,\omega)\, U_0(q)\, \Pi(q,\omega) \cdots$$

$$+ \Pi(q,\omega) U_0\, \Pi(q,\omega)\, U_0\, \Pi(q,\omega) + \cdots$$

$$= \Pi(q,\omega) + \Pi(q,\omega)\, U_0(q)\, D(q,\omega)$$

$$\therefore D(q,\omega) = \frac{\Pi(q,\omega)}{1 - \Pi(q,\omega) U_0} \quad --- \quad (72)$$

Similarly, $V_0 D(q,\omega) = \Pi(q,\omega)\left[U_0 + U_0 \Pi V_0 + U_0 \Pi V_0 \Pi V_0 + \cdots\right]$

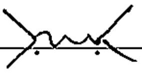
$$= \Pi(q,\omega) V(q,\omega) \quad -- \quad (73)$$

From eq.(71), it is clear that the screening is determined by $\Pi(q,\omega)$, reflected in the dielectric function.

Note that from eq.(72), one gets

$$1 + U_0 D = 1 + \frac{\Pi U_0}{1 - \Pi U_0} = \frac{1}{1 - \Pi U_0} = \frac{1}{\epsilon(q,\omega)}$$

which is eq.(P) with χ^R bare replaced by D !

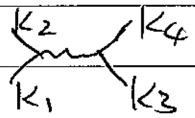
lines ∵ Each  contributes 4 solid lines.

∴ Total — lines = $4n$

∵ Each g_k^0 is obtained by connecting two — lines.

∴ Number of g_k^0 in nth order $= \frac{4n-2}{2}$ ← two external lines.

$= 2n-1$ --- (74)

Now each interaction  has a momentum conservation $\delta(k_1+k_2+k_3+k_4)$, which elliminates one momentum. Overally, there is a δ function associated with Σ. ∴ Total # of momentum conservation requirements $= n-1$

Each g_k^0 carries one momentum. After elliminating the momentum conservation, the remaining momentum are those in the integrals.

∴ Number of internal momentum to be integrated

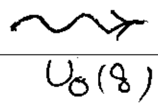
$= (2n-1) - (n-1) = n$ --- (75)

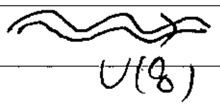
For nth order, number of $V_0(q) = n$ --- (76)

We can rescale k by k_F ($k \to k/k_F$), $i\omega_n$ (or ξ_k) by k_F^2, $\frac{1}{\beta}$ by k_F^2 (∵ $\omega_n = \frac{2\pi n}{\beta}$, $\frac{1}{\beta} \sim \omega_n$)

Self-energy and random phase approximation

$U(q)$ is the total potential, sometimes called renormalized potential, which also contributes to the self energy of the electron.

Diagramatically, one can replace any 

in the perturbation theory by 

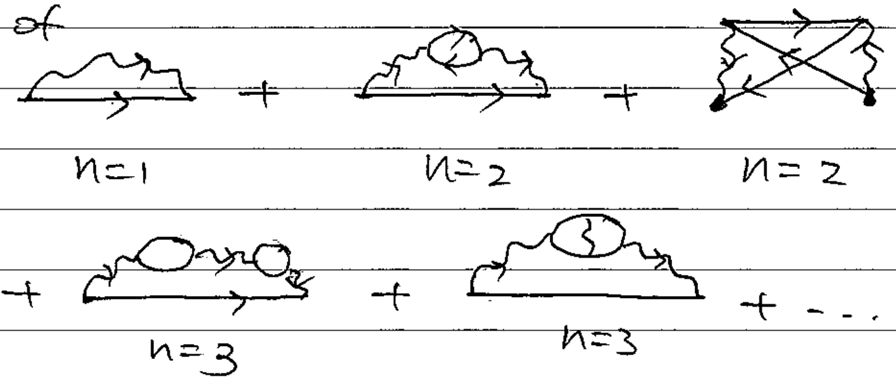
.

Now, with so many diagrams, which ones contribute most importantly?

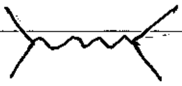
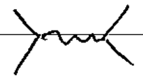
To answer this question, we shall examine the self-energy $\Sigma(k, i\omega)$ more closely.

(i) density dependence

First, lower orders of

$\Sigma(k, i\omega) =$ 

due to $V_0(q)$ (without contribution from phonons).

For n th order, there are n  and from n , one forms Σ with two external

∵ $V_0(q) = \frac{4\pi e^2}{q^2}$ ∴ $U_0(q)$ Contributes k_F^{-2}

$$g_k^0 = \frac{1}{i\omega_n - \xi_k} \propto k_F^{-2}$$

$\frac{1}{\beta}\sum_{i\omega_n}$ goes with each internal line

$\propto k_F^{+2}$

∴ For nth order, one gets its k_F

$$\text{dependence} = \underbrace{(k_F^{-2})^n}_{U_0(q)} \underbrace{(k_F^{-2})^{2n-1}}_{g_k^0}$$

$$\times \underbrace{(k_F^{5})^n}_{\frac{1}{\beta}\sum_{i\omega_n}\int\frac{d^3k}{(2\pi)^3}\ \text{internal line integral \& frequency sum}}$$

$$= k_F^{-(n-2)} \quad \text{-- (77)}$$

Since $\frac{4\pi}{3}k_F^3 \times 2 = n_e$, ∴ $k_F \propto n_e^{\frac{1}{3}} \propto r_s$.

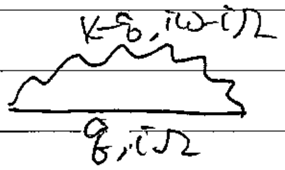
Eq. (77) implies that in high densities, lower orders (small n) dominate.

(ii) degree of divergence

If one adopts the original (bare) Coulomb interaction, $V_0(q) = \frac{4\pi e^2}{q^2}$, some of diagrams are not well defined

Furthermore, the dominant contribution comes from the region of $q \simeq 0$ for $v_0(q) = \frac{4\pi e^2}{q^2}$.

For example



$$= \frac{(-1)}{\beta} \sum_{i\Omega} \int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{(k-q)^2} \frac{1}{i\Omega - \xi_q}$$

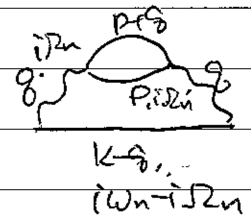
$$\sum_{i\Omega} \frac{1}{i\Omega - \xi_q} = n_F(\xi_q)$$

$\therefore$

$$= \frac{-1}{\beta} \int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{(k-q)^2} n_F(\xi_q)$$

Clearly, the dominant contribution comes from the region $q \simeq k$.

Similarly,



Fermion loop $\downarrow$

$$= \frac{(-1)}{(\beta V)^2} \sum_{\sigma' p q} \sum_{\substack{i\Omega_n \\ i\Omega_n'}} \left(\frac{4\pi e^2}{q^2}\right)^2 \mathcal{G}^0(p, i\Omega_n') \mathcal{G}^0(p+q, i\Omega_n + i\Omega_n')$$

$$\times \mathcal{G}^0(k-q, i\omega_n - i\Omega_n)$$

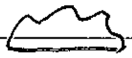
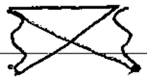
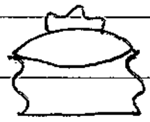
$$= \frac{1}{\beta} \sum_{i\Omega_n} \int \frac{d^3q}{(2\pi)^3} \frac{(4\pi e^2)^2}{q^4} \left(+\chi_0(q, i\Omega_n)\right) \mathcal{G}^0(k-q, i\omega_n - i\Omega_n)$$

which shows divergent behavior near $q \simeq 0$.

In general, it is clear that when all v_0 in a diagram have the same momentum q, these diagrams are most divergent! One can define the degree of divergence of a diagram Σ by δ

δ = # of interaction lines that can have the same momentum q.

The followings are degrees of divergence for a few lower order terms :

	$n=1$	$n=2$	$n=3$
$\delta=1$			 
$\delta=2$	-		 
$\delta=3$	-	-	

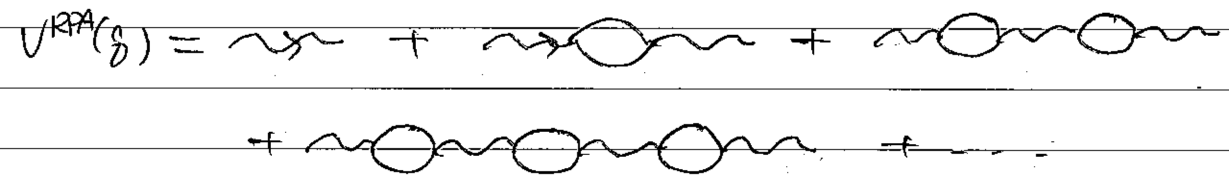
Clearly, one sees that for a given n, the dominant contribution is the case when $\delta = n$.

These diagrams are composed by rings and called ring diagrams. Consideration of only ring diagrams and their summation is called random phase approximation (RPA).

The random phase approximation was first introduced by David Bohm and David Pine by considering phases $e^{iq\cdot r_i}$ of each vertex and is now commonly used for describing dynamical linear response of electronic systems.

In RPA, one approximates

$V^{RPA}(q) =$



$$= \frac{V_0(q)}{1-V_0(q)\chi_0} = \frac{4\pi e^2}{q^2-4\pi e^2\chi_0(q,i\omega)} \cdots (78)$$

Thomas - Fermi screening & Friedel oscillation

In the $q \to 0$, $i\omega_n \to 0+i0^+$, (static & long-wave limit), $U^{RPA}(q,0) \to \frac{4\pi e^2}{q^2+k_s^2}$

with $k_s^2 \equiv -4\pi e^2 \chi_0(0,0)$. This corresponds to the Thomas - Fermi screening approximation.

∵ The induced charge $\delta\langle\hat{n}(k,\omega)\rangle = D(k,\omega)\, e\phi_{ext}(k,\omega)$

∴ For a point impurity charge, $e\phi_{ext} = \frac{-4\pi e^2 Z}{k^2}$, Ze = impurity charge

one gets $\delta\langle\hat{n}(k)\rangle = D(k,0)\underbrace{\frac{-4\pi e^2 Z}{k^2}}_{V_0} \underset{*}{=} \frac{-Z V_0 \Pi}{1-V_0\Pi} = \frac{-Z V_0\chi_0}{1-V_0\chi_0}$ (92)

$$\therefore \delta\langle n^{RPA}\rangle = \frac{4\pi e^2\chi_0(q,0)Z}{q^2-4\pi e^2\chi_0(q,0)} \approx \frac{+k_s^2 Z}{q^2+k_s^2}$$

In the Thomas-Fermi approximation, one considers the pressure of free electron gas at T=0

$$PV=\frac{2}{3}E \Rightarrow p=\frac{2}{5}\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}n^{5/3}$$

The balance between local p & $\vec{E}$ gives

$$-\nabla p-en\vec{E} = 0 \Rightarrow \frac{2}{3}\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}\frac{1}{n^{1/3}}\nabla n=e\nabla\phi \quad (79)$$

Now. $\nabla\cdot\vec{E}=-\nabla^2\phi=4\pi Ze\delta(\vec{r})-4\pi e\underbrace{(n-n_0)}_{\delta n}$ (80)

n_0 = electron density at equilibrium

Eq. (79) implies $\frac{2}{3}\frac{\hbar^2k_F^2}{2m}\frac{1}{n_0}\nabla\delta n=e\nabla\phi$

Taking $\nabla\cdot$ and using eq. (80), one gets

$$(\nabla^2-q_{TF}^2)\delta n=-Zq_{TF}^2\delta(\vec{r})$$

where $q_{TF}=\frac{6\pi n_0e^2}{\epsilon_F^0}=6\pi e^2\times\frac{2m}{\hbar^2}(3\pi^2)^{-\frac{2}{3}}n_0^{1/3}$

Hence $\delta n(q)=\frac{Zq_{TF}^2}{q^2+q_{TF}^2}$

Therefore, RPA results in Thomas-Fermi approximation with k_s^2 replacing q_{TF}^2.

For $k_BT \ll \epsilon_F$, $\therefore \chi_0(q,0)=2\int\frac{d^3k}{(2\pi)^3}\frac{n_F(\xi_{k+q})-n_F(\xi_k)}{\xi_{k+q}-\xi_k+i0^+}$

$$\chi_0(q\to 0, 0) = 2\int \frac{d^3k}{(2\pi)^3} \frac{\cancel{(\xi_{k+q}-\xi_k)}\,\frac{dn_F(\xi_k)}{d\xi_k}}{\cancel{(\xi_{k+q}-\xi_k)}}$$

$$= 2\int \frac{d^3k}{(2\pi)^3} -\delta(\varepsilon_F - \varepsilon_k) = -\underset{\substack{\uparrow \\ \text{density of states} \\ \text{at } \varepsilon_F}}{N(\varepsilon_F)}$$

$$\therefore k_s^2 = -4\pi e^2 \chi_0(0,0) = 4\pi e^2 N(\varepsilon_F)$$

$$N(\varepsilon_F) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon_F^{1/2} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left(\frac{\hbar^2}{2m}\right)^{\frac{1}{2}} \times (3\pi^2)^{\frac{1}{3}} \times n_0^{\frac{1}{3}}$$

One finds $k_s^2 = q_{TF}^2$.

The Thomas-Fermi result is only an approximated result of the RPA summation.

It implies that the potential form after screening is Yukawa potential

$$V_{TF}(r) = \frac{e^2}{r}\, e^{-k_s r}$$

i.e. the induced charge $\delta\langle\rho\rangle = -\frac{Zek_s^2}{4\pi r} e^{-k_s r}$ approaches zero as $r\to\infty$

Using the exact form of χ_0, however, the induced charge density actually oscillates and decays in power law.

For this purpose, one needs to evaluate χ_0 exactly. This was done before, we have

$$\delta\langle\rho(q)\rangle = (-e)\langle\delta n(q)\rangle$$

$$= Ze\,\frac{4\pi e^2\chi_0(q,0)}{q^2-4\pi e^2\chi_0(q,0)}$$

$$-4\pi e^2\chi_0(q,0) = (4\pi e^2)\times\frac{mk_F}{\hbar^2}\frac{1}{2\pi^2}\left(-1+\frac{1}{q/k_F}\left(1-\frac{1}{4}\frac{q^2}{k_F^2}\right)\ln\left|\frac{1-\frac{q}{2k_F}}{1+\frac{q}{2k_F}}\right|\right)$$

$$\|$$

$$\mathrm{Re}\,\chi_0(q,0)\ (\mathrm{Im}\,\chi_0(q,0)=0)$$

$$= q_{FT}^2\, g(q/k_F) \qquad g(x)=\frac{1}{2}-\frac{1}{2x}\left(1-\frac{x^2}{4}\right)\ln\left|\frac{1-\frac{1}{2}x}{1+\frac{1}{2}x}\right|,\ x=q/k_F$$

$$\therefore\ \delta\langle\rho(q)\rangle = -Ze\,\frac{q_{FT}^2\, g(q/k_F)}{q^2+q_{FT}^2\, g(q/k_F)}$$

$$\delta\langle\rho_{RPA}(\vec r)\rangle = -Ze\int\frac{d^3q}{(2\pi)^3}\,e^{i\vec q\cdot\vec r}\,\frac{q_{FT}^2\, g(q/k_F)}{q^2+q_{FT}^2\, g(q/k_F)}$$

$$= -\frac{Ze}{2\pi^2 r}\int_0^\infty dq\, q\sin qr\,\frac{q_{FT}^2\, g(q/k_F)}{q^2+q_{FT}^2\, g(q/k_F)} \cdots (\rho_1)$$

$$\because\ g(-x)=\frac{1}{2}+\frac{1}{2x}\left(1-x^2/4\right)\ln\left|\frac{1+\frac{x}{2}}{1-x/2}\right| = \frac{1}{2}-\frac{1}{2x}\left(1-x^2/4\right)\ln\left|\frac{1-x/2}{1+x/2}\right|$$

$$= g(x)$$

∴ The integrand in eq (ρ_1) is even in q, one can rewrite $\int_0^\infty dq$ as $\int_{-\infty}^{\infty} dq$.

$$\therefore\ \delta\langle\rho_{RPA}(r)\rangle = \frac{Ze}{4\pi i r}\int_{-\infty}^{\infty} q\,dq\, e^{i\vec q\cdot\vec r}\left[\frac{q^2}{q^2+q_{FT}^2\, g(q/q_{FT})}-1\right] \cdots (\rho_2)$$

In eq. (P2), the integrand has singularities

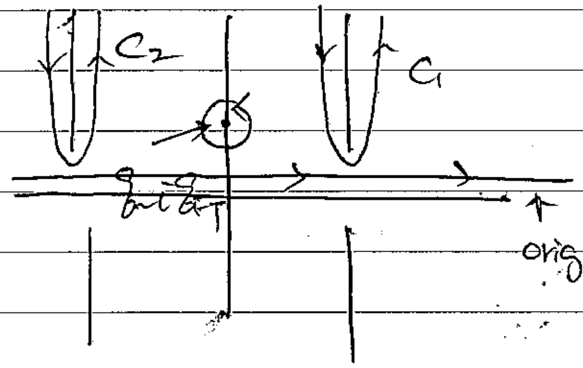
(i) a pole roughly at $q \simeq i q_{FT}$

(ii) Branch cut due to Log.

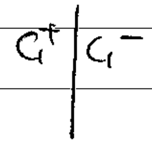
$$\ln\left|\frac{1-x/2}{1+x/2}\right| = \frac{1}{2}\lim_{\eta\to 0}\ln\frac{(q-2k_F)^2+\eta^2}{(q+2k_F)^2+\eta^2}$$

Branch of $\ln z = \ln|z| + i\theta \quad -3\pi/2 < \theta \le \pi/2$

∴ One can replace the original integral by



$$\int_{C_1} + \int_{C_2} + \int_{pole}$$



across C_1 $$\ln\frac{(q-2k_F)^2+\eta^2}{(q+2k_F)^2+\eta^2}\Big|_{C_1^+} = \ln(q-2k_F)^2 + i(-3\pi/2) - \ln|q+2k_F|^2 - i0$$

$$\ln \quad '' \quad \Big|_{C_1^-} = \ln|q-2k_F|^2 + i\pi/2 - \ln|q+2k_F|^2 - i0$$

$$\therefore \frac{1}{2}\underset{C_1^- - C_1^+}{\Delta}\ln\frac{(q-2k_F)^2+\eta^2}{(q+2k_F)^2+\eta^2} = i\pi$$

∵ e^{iqx} along C_1 $\underset{q = 2k_F + iv}{=}$ $e^{i2k_F x}\, e^{-vx}$ is decaying
$v > 0$

e^{iqx} along C_2 = $e^{-i2k_F x}\, e^{-ux}$ $\quad q = -2k_F x + iu$

One may replace $\left[\frac{q^2}{q^2+q_{FT}^2\, g(q/k_F)}-1\right]q$

$$=\frac{-q_{FT}^2\, g(q/k_F)}{q^2+q_{FT}^2\, g(q/k_F)}\times q$$

$x=q/k_F=2k_F/k_F+i\frac{v}{k_F}$

$$\text{by } 2k_F\times\frac{-q_{FT}^2}{(2k_F)^2+\frac{q_{FT}^2}{4}}\times\left[\frac{1}{2}-\underbrace{\frac{1}{2}\left(1-\frac{x^2}{4}\right)}_{\substack{\shortparallel\\ \frac{1}{2}\left(-4i\frac{v}{k_F}\right)}}\Delta\underbrace{\frac{1}{2}\ln\frac{(q-2k_F)^2+\eta^2}{(q+2k_F)^2+\eta^2}}_{\substack{\shortparallel\\ i\pi}}\right]$$

∴ C_1 integral

$$\sim \text{Constant}>0\cdot\frac{Ze}{4\pi i x}\, e^{2ik_F x}\int_\eta^\infty v\, e^{-vx}\underbrace{dq}_{\substack{\shortparallel\\ i\,dv}}$$

Similarly, C_2 integral

$$\sim \text{constant}\cdot\frac{Ze}{4\pi i x}\, e^{-2ik_F x}\int_\eta^\infty u\, e^{-ux}\, i\,du$$

Combining C_1 & C_2, one gets

$$\delta\langle\rho_{RPA}(r)\rangle\sim Ze\cdot\text{positive constant}\cdot\frac{\cos 2k_F r}{r^3}\quad (83)$$

Eq. (83) implies that instead of decaying implied by the Thomas-Fermi approximation, $\delta\langle\rho_{RPA}(r)\rangle$ actually oscillates and decay in power law. This was first suggested by Friedel, such Friedel oscillations have been observed in dilute alloys.

Stoner criterion and ferromagnetic instability

The RPA can be also applied to investigate magnetic instability.

We shall take the Hubbard model as an example. It may seem that the Hubbard model does not support ferromagnetism. Howerever, let $H_U = U\sum_i n_{i\uparrow}n_{i\downarrow}$,

It is possible to rewrite H_U as follows:

$$S_x = \frac{1}{2}(C_\uparrow^+ C_\downarrow + C_\downarrow^+ C_\uparrow) \qquad (\hbar = 1)$$

$$S_y = \frac{1}{2i}(C_\uparrow^+ C_\downarrow - C_\downarrow^+ C_\uparrow)$$

$$S_z = \frac{1}{2}(n_\uparrow - n_\downarrow)$$

$$\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = \frac{1}{4}(C_\uparrow^+ C_\downarrow + C_\downarrow^+ C_\uparrow)^2 - \frac{1}{4}(C_\uparrow^+ C_\downarrow - C_\downarrow^+ C_\uparrow)^2 + \frac{1}{4}(n_\uparrow - n_\downarrow)^2$$

$$= \frac{1}{2}(\underbrace{C_\uparrow^+ C_\downarrow C_\downarrow^+ C_\uparrow}_{\substack{\parallel \\ n_\uparrow(1-n_\downarrow)}} + \underbrace{C_\downarrow^+ C_\uparrow C_\uparrow^+ C_\downarrow}_{\substack{\parallel \\ n_\downarrow(1-n_\uparrow)}}) + \frac{1}{4}(\underbrace{n_\uparrow^2}_{\substack{\parallel \\ n_\uparrow}} - 2n_\uparrow n_\downarrow + \underbrace{n_\downarrow^2}_{\substack{\parallel \\ n_\downarrow}})$$

$$= \frac{3}{4}n - \frac{3}{2}n_\uparrow n_\downarrow$$

$$\therefore n_\uparrow n_\downarrow = \frac{1}{2}n - \frac{2}{3}\vec{S}^2$$

$$\therefore\ H_U = \frac{U}{2}\sum_i n_i - \frac{2}{3}U\sum_i \vec{S_i}\cdot\vec{S_i}$$

The first term shifts the chemical potential.

Therefore the interaction $H_{int} = \underbrace{\frac{-2}{3}U}_{J}\sum_i \vec{S_i}\cdot\vec{S_i}$

is in terms of spin-spin interaction.

$J = \frac{-2U}{3}$ is called exchange coupling.

$$\because\ \vec{S_i}\cdot\vec{S_i} = \frac{1}{2}(S_i^+ S_i^- + S_i^- S_i^+) + S_i^z S_i^z$$

By assuming isotropic, we have the bubble in the RPA approximation for S^+ & S^- be $\frac{1}{2}\chi_0$. $S_i^z S_i^z$ contributes equally.

We get the dynamical spin susceptibility in the RPA approximation as

$$\frac{1}{2}\chi^{RPA} = \chi^{RPA}_{+-}(q,\omega) = \frac{\chi_0^{+-}}{1-J\chi_0^{+-}}$$

$$= \frac{1}{2}\frac{\chi_0}{1+U/3\,\chi_0}$$

$$\therefore\ \chi^{RPA} = \frac{\chi_0}{1+U/3\,\chi_0} \quad \cdots\ (84)$$

One sees that the denominator in χ^{RPA} may vanish. Suppose it happens at Q, $\omega=0$, it indicates that one gets huge magnetic response of $\vec{S}(Q,0)$. Therefore, the system tends to develope spin density wave at $\vec{Q}$.

When $\vec{Q}=0$, $\because$ $\chi_0 \underset{\substack{\uparrow \\ \text{at } T=0}}{=} -N(\varepsilon_F)$,

The vanishing of denominator in eq. (84) implies

$$1 = \underbrace{\frac{2}{3}U}_{I\ \text{(exchange strength)}} N(\varepsilon_F) \quad \cdots \text{(85)}$$

Eq. (85) is the Stoner criterion for ferromagnetic instability.

There are situations in which exchange terms happen to be between nearest neighbour with $J>0$ $\quad J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$. For square lattices, after Fourier transformation, it becomes

$$J\sum_q(\cos q_x+\cos q_y)\,\vec{S}_q\cdot\vec{S}_{-q}$$

J becomes $J(q)=J(\cos q_x+\cos q_y)$.

In this case, $\chi^{RPA} = \dfrac{\chi_0}{1-\frac{1}{2}J(q)\chi_0}$ $\cdots$ (86)

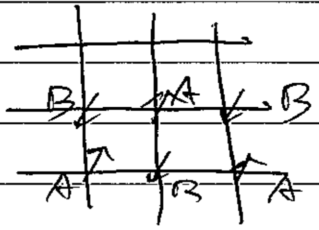
Hence at $q=0$, $J(q)>0$ ∵ $\chi_0<0$

there is no ferromagnetic instability.

However, at $q=(\pi,\pi)$, $J(q)<0$. In this case, the instability may occur with the criterion

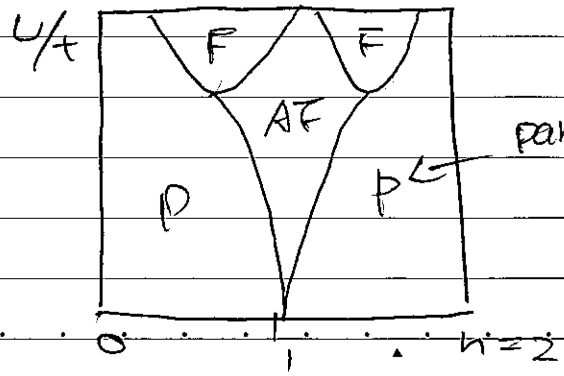
$$1 = \frac{1}{2}J(\pi,\pi)\,\chi_0(\pi,\pi)$$
$$= -J\chi_0(\pi,\pi).$$

When this happens, the spin varies with the following pattern



$$∵ \quad e^{i\vec{q}\cdot\vec{r}} = e^{i(\pi x+\pi y)} = (-1)^{x+y} = +1 \text{ for A sublattice}$$
$$= -1 \text{ for B}.$$

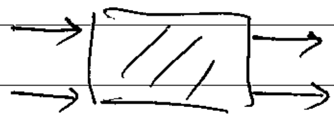
Such instability is called antiferromagnetic (AF) instability. This indeed happens for certain parameter regime of the Hubbard model.



(T=0) mean-field phase diagram of the Hubbard model.

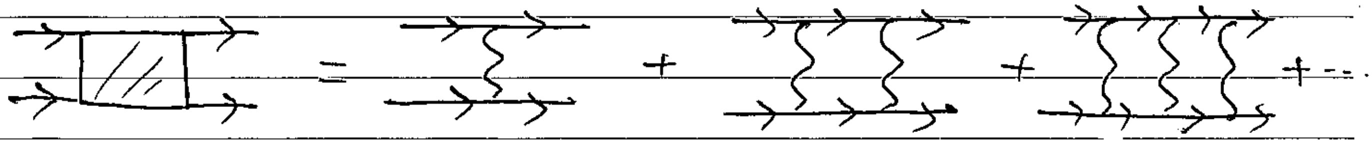
Ladder diagram and the Cooper instability

The bubble diagrams in RPA are not exactly two-particle propagators, instead, they can be viewed as particle-hole propagators. To have two-particle propagators, two particles have to come in (enter) and two particles come out as follows

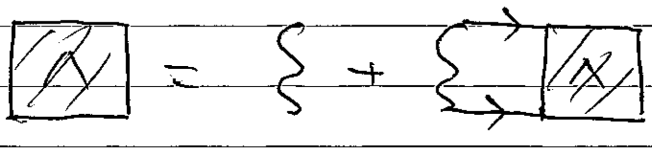


particle-particle channel.

The simplest such diagrams are ladder diagrams, which we have seen in investigation of Anderson localization.



These ladder diagrams can be resummed as follows



--- (86)

Eq. (86) is the same as the equation for Γ in the problem of localization, but here Λ is the effective interaction!

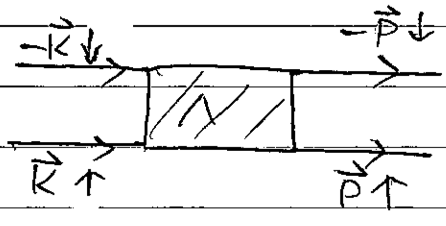
Just as the ferromagnetic instability in the RPA, there is also an instability associated with the ladder diagrams. This occurs when $V_0(q)$ is renormalized and becomes negative.

$$V_0(q) \longrightarrow U_{eff}^{\overset{\swarrow \text{Phonon}}{RPA}} \cong -V \qquad |i\omega_n| < \omega_D$$

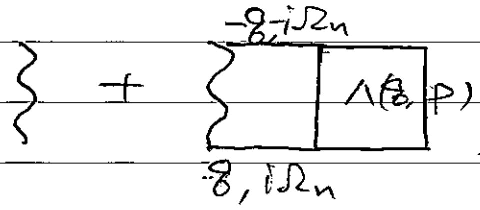
$$\simeq 0 \qquad |i\omega_n| > \omega_D$$

This was pointed out by Cooper but in this framework.

In this case, electrons of opposite spins enter with their center of momentum being zero. as shown in below:



$\therefore \Lambda = \Lambda(\vec{k},\vec{p}) =$



$$= -U_{eff}^{RPA} + \frac{1}{V\beta}\sum_{q}\sum_{i\Omega_n}\left(-U_{eff}^{RPA}\right) g_\uparrow^0(q,i\Omega_n)\, g_\downarrow^0(-q,-i\Omega_n)$$

$$\times \Lambda(\vec{q},\vec{p}) \quad \text{---} \; ⑧⑦$$

Setting $-V_{eff}^{RPA} = U$, equation (87) becomes

$$\Lambda(k,p) = U + \frac{U}{\beta} \sum_{i\Omega_n}^{\omega_D} \frac{1}{V} \sum_{q} g_{\uparrow}^{0}(q, i\Omega_n) g_{\downarrow}^{0}(-q, -i\Omega_n)$$

$$\times \Lambda(q, p) \quad \text{--} (88)$$

Since right hand side of (88) doesn't depend on k, $\therefore$ $\Lambda(k,p) = \Lambda(p)$. Hence $\Lambda(q,p) = \Lambda(p)$

Eq. (88) can be solved, we find

$$\Lambda(p) = \underset{\substack{\uparrow \\ p \text{ independent}}}{\Lambda} = \frac{U}{1 - \frac{U}{\beta} \sum_{|\Omega_n| < \omega_D} \frac{1}{V} \sum_{q} g_{\uparrow}^{0}(q, i\Omega_n) g_{\downarrow}^{0}(-q, -i\Omega_n)}$$

$$\text{--} (89)$$

In eq. (89), one sees that it is possible for an instability to occur when the denominator vanishes. When this happens, Λ becomes $-\infty$ (approach from above, denominator $= 0^{-}$) as T is lowering down! ($\frac{1}{\beta} = k_B T$)

In other words, the effective interaction Λ becomes $-\infty$ so that a bound state of two electrons can form. This is known as the Cooper instability.

Note that the Cooper instability is not the same as solving two-particles in the presence of an attractive potential in the two-particle Schrödinger equation. The presence of other electrons is crucial and that is why the temperature enters!

The instability occurs at a particular temperature T_c, $\beta_c = \frac{1}{k_B T_c}$. From eq. (89), one gets

$$1 = \frac{V}{\beta_c} \sum_{|i\Omega_n|<\omega_D} \frac{1}{V} \sum_q g_\uparrow^0(q, i\Omega_n)\, g_\downarrow^0(-q, -i\Omega_n)$$

$$= \frac{V}{\beta_c} \sum_{\substack{|i\Omega_n| \\ <\omega_D}} \frac{1}{V} \sum_q \frac{1}{i\Omega_n - \xi_q} \, \frac{1}{-i\Omega_n - \underset{\underset{\xi_{-q}}{\shortparallel}}{\xi_q}}$$

$$= \frac{V}{\beta_c} \sum_{|i\Omega_n|<\omega_D} \int_{-\infty}^{\infty} d\xi \, \frac{1}{\Omega_n^2 + \xi^2} \, \underbrace{N(\xi)}_{\text{density of state}}/2 \leftarrow \text{only one spin}$$

$\because \omega_D \ll \varepsilon_F$ $\therefore$ one can approximate

$$N(\xi) = N(0) = N(\varepsilon_F)$$

One gets $1 = \frac{V}{\beta_c} \sum_{|i\Omega_n|<\omega_D} \frac{N(\varepsilon_F)}{2} \int_{-\infty}^{\infty} \frac{d\xi}{\xi^2 + \Omega_n^2}$

Performing the integral, one has

$$\int_{-\infty}^{\infty}\frac{d\xi}{\xi^2+\Omega_n^2} = \frac{\pi}{|\Omega_n|}$$

$$\therefore \quad 1 = \frac{VN(\varepsilon_F)\pi}{2\beta_c}\sum_{\substack{|i\Omega_n|\\<\omega_D}}\frac{1}{|\Omega_n|}$$

$$= \frac{1}{2}VN(\varepsilon_F)\left[\sum_{n=0}^{\frac{1}{2\pi}\beta_c\omega_D}\frac{1}{n+1/2} - 2\right] \quad \text{--}\ (88)$$

Where we made use of $\Omega_n = \frac{2\pi}{\beta_c}(n+1/2)$

And coverted $n=-1,-2\ldots$ n to $1, 2, \ldots$

($n=0$ is doubly counted, $\therefore -2$ counts for it).

Now, using the identity

$$\sum_{n=0}^{\frac{1}{2\pi}\beta_c\omega_D}\frac{1}{n+1/2} - 2 \approx \ln 4\frac{\beta_c\omega_D}{2\pi}$$

for $\beta_c\omega_D >> 1$

$$\therefore \quad 1 \cong \frac{VN(\varepsilon_F)}{2}\ln\frac{4\beta_c\omega_D}{2\pi}$$

$$k_BT_c \simeq \overset{\uparrow}{\hbar}\omega_D\, e^{-\frac{2}{VN(\varepsilon_F)}}$$

put back $\hbar$

Which shows similar form of critical coupling strength for CDW & SDW. Typical $\hbar\omega_D \sim 100K$, the exponential form in $1/V$ however can reduce T_c to about 1K.